



OVERSEA CORPORATIVE EDUCATION REPORT

Process Analysis and Process Intensification of Industrial Scale Process

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Abstract

Chemical industry is facing a new model when we thought about Process Intensification as a great tool to find innovative and more sustainable solutions to chemical manufacturing and processing. Even a mature technology, as urea production, can be improved generating not only just economic advantages, but also a reduction in their environmental impact, ensuring energy-saving and an increase in production. The proposal presented here is to apply a sustainable process synthesis-intensification method (Babi et al, 2015), with the associated industrial work-flow and data-flow, consisting of two stages: (1) Base case design analysis: identify a base-case in terms of operational feasibility, economics, sustainable measures and life cycle assessment factors to identify process bottleneck and define targets for the next step; (2) Innovation: generation of more sustainable framework processes through a phenomena-based process. In this work, an urea plant was modelled and simulated in a commercial process simulator. Economic and sustainability analysis were performed and the main hot-spots were identified. Process intensification at phenomena-level was employed to obtain a more sustainable intensified process flowsheets. The results show that economic, social and environmental factors can be improved.

Keywords: urea production, process analysis, process intensification, sustainable solutions.

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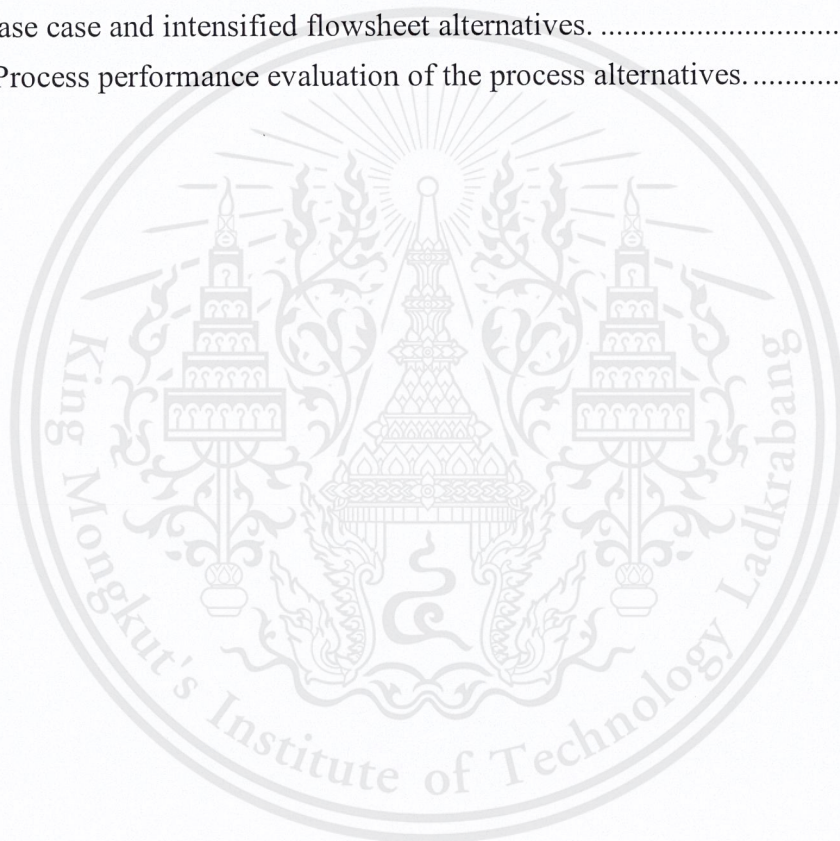


Table of Contents

	Page
Abstract.....	i
Acknowledgements	ii
Table of Contents	iii
List of Figures.....	iv
List of Tables.....	v
Nomenclature.....	vi
Chapter I Introduction	1
1.1 Introduction	1
1.2 Objectives	1
1.3 Scopes of work	2
1.4 Expected outputs	2
Chapter II Literature Review.....	3
2.1 Process synthesis	3
2.2 Intensification of processes	3
2.3 Stages of process intensification.....	4
2.4 Urea production process	6
Chapter III Research Methodology	7
3.1 Part 1: Base case design analysis.....	7
3.2 Part 2: Sustainable design or innovation	9
Chapter IV Results and Discussion	11
4.1 Case study.....	11
4.2 Part 1: Base case design analysis.....	11
4.3 Part 2: Sustainable design or innovation	15
Chapter V Conclusion	24
5.1 Summary.....	24
5.2 Recommendations for further research.....	24
References	25
Appendix	27
Biography	42

List of Figures

	Page
Figure 1: The concept of process synthesis-intensification framework.	5
Figure 2: Simplified block diagram for the urea production process	6
Figure 3: The overall framework for this project.	7
Figure 4: Calculated mass (kg/h) and energy (GJ/h) balance for the base case design.....	11
Figure 5: Base case simulation flowsheet	12
Figure 6: Economic analysis and LCA analysis for the base case design.....	14
Figure 7: The task-based flowsheet of the base case design for urea production process. .	16
Figure 8: Phenomena based flowsheet of the base case design.....	16
Figure 9: Base case and intensified flowsheet alternatives.	21
Figure 10: Process performance evaluation of the process alternatives.....	23



List of Tables

	Page
Table 1. The 4 most critical paths in the base case design	13
Table 2. Sustainability metrics for the base case design.	13
Table 3. Main identified bottlenecks with sustainability, economic and LCA analysis.	15
Table 4. Identified process hot-spots for the base case design.....	15
Table 5. Binary ratio matrix for a set of selected properties.	17
Table 6. List of selected (desirable) PBBs linked to the identified tasks.	18
Table 7. Partial list of feasible SPBs..	19
Table 8. Generation of hybrid/intensified unit operations from combination of PBBs.	20
Table 9. Comparison of the base case design and the alternative design.....	22



Nomenclature

2phM	2-phase mixing
AF	Accumulation factor
Carb	Ammonium carbamate
C-	Compressor
D	Dividing
EWC	Energy waste cost
E-	Heat exchanger
eq.	Equivalent
GWP	Global warming potential
HTPI	Human toxicity potential by ingestion
H/C	Heating/Cooling
IP	Intensification of processes
L	Liquid
LCA	Life cycle assessment
LD ₅₀	lethal concentration
M	Mixing
MVA	Material value added
MW	Molecular weight
NSPB _{max}	Total number of possible SPBs
nPBB	Total number of phenomena building blocks
nPBB _D	Total number of dividing phenomena
nPBB _E	Total number of energy transfer phenomena
nPBB _M	Total number of mixing phenomena
PBBs	Phenomena building blocks
PC	Phase contact
PT	Phase transition
PS	Phase separation
P-	Pump
R	Reaction
RG	Radius of gyration
RM	Raw materials
R-	Reactor
Rc-	Reactor-condenser
SolPar	Solubility parameter
SP	Process synthesis
SPBs	Simultaneous phenomena building blocks
TVA	Total value added
T-	Tower or column
Tc-	Column-condenser
Tr-	Column-reboiler
Tb	Boiling temperature
Tm	Melting temperature
V	Vapor
VdW	Van der Waals volume
VM	Molar volume
VP	Vapor pressure

Chapter I

Introduction

1.1 Introduction

In the chemical industry, process improvements related to the development of sustainable technologies and the efficient use of available resources are necessary in order to achieve reductions in energy consumption, environmental impact and also the cost of production. Process improvements are usually obtained through an evolutionary approach, where knowledge gained from process understanding along with specialized knowledge in process engineering is applied (Babi et al, 2015).

To identify hot spots of a process, economic, sustainability and Life Cycle Assessment (LCA) analyses can be employed and then targets for overcoming these “hot-spots” are defined. Process Intensification study in order to improved values of a set of targeted performance parameters and achieve a more sustainable process. Process intensification is defined as improvements of a process at unit operational, functional and/or phenomena levels that can be obtained by integration of unit operations, integration of functions and phenomena’s or targeted enhancement of the phenomena for a set of target operations (Lutze et al., 2013).

This paper use as base case the urea production process. A simulation model was built in a commercial software and industrial data were used to validate it. Economic analysis was performed using the tools proposed by (Saengwirun, 2011). Sustainability analysis was accomplished following (Carvalho et al, 2008) and (Tallis, 2002) and for LCA analysis it was used UK Government GHG conversion factors the tools proposed by (Tallis, 2002). Process Intensification was performed using a multi-stage framework according to (Babi et al, 2015).

1.2 Objectives

- To identify process bottlenecks (process hot-spots) of industrial scale process using three analyses (Economic, Sustainability and LCA analyses).
- To generate more sustainable process alternatives using concept of process synthesis-intensification at phenomena-level.

1.3 Scopes of work

- Base case process is the urea production process in industrial scale.
- For LCA analysis considers only carbon footprint, global warming potential and human toxicity potential.
- For economic analysis considers only utility cost.

1.4 Expected outputs

Hot spots of base case design of urea production process will be identified then will be eliminated or reduced by using concept of process synthesis-intensification at phenomena-level generate more sustainable alternative.



Chapter II

Literature Review

2.1 Process synthesis

The goal of Process Synthesis is to find the best processing route, among the many alternatives, to convert raw materials into specific products, subject to pre-defined performance criteria. Thus, Process Synthesis involves the analysis of the problem, the generation and evaluation of alternatives until the best option can be identified. In this way, solving a problem of process synthesis is usually accomplished through three methods:

- (a) Heuristic methods: based on rules defined from the knowledge of the process.
- (b) Methods based on mathematical programming: the most suitable flowchart is determined from a network for optimization of the structure. This method is widely used when the system is well defined and a large number of alternatives can be considered.
- (c) Hybrid methods: make use of both heuristic rules based on process knowledge and programming of mathematical models.

The main function of these three methods is to reduce the search space of alternatives so that the problem has an efficient solution in the shortest possible time (Babi et al, 2015)

2.2 Intensification of processes

The main focus of the Process Synthesis is the study of the process in the scale of unitary operations. Process Intensification involves the study of task scales and phenomena. IP has received increasing attention because of its innovative potential and its more sustainable project proposals. Thus, in addition to the traditional resolutions with optimal processing routes, we can also count on the potential use of hybrid / intensified equipment, whether new or already well established in the market, or in the adaptation of existing processes. Thus, the studies of Synthesis and Process Intensification bring greater advantages when they are carried out concomitantly in the evaluation of a process. Many IP definitions have been proposed in the last two decades (Huther et al, 2005). Here are just a few:

"IP is a strategy of reducing chemical plants while maintaining the same productive capacity" (Cross et al, 1986)

"IP is all chemical engineering development that leads to cleaner, more sustainable and energy efficient technology." (Staniewicz et al, 2000).

"IP is a revolutionary approach to designing, developing and implementing plants and processes. Provides a chemical process with the ideal environment for better results, cleaner, safer and cheaper products and processes. IP not only exchanges old equipment for new, enhanced and more efficient equipment, it challenges business models, opening up opportunities for patentable chemical products and processes. "(BHR Group apud Keil, 2007).

"IP is a holistic approach, starting with an analysis of economic constraints followed by a selection or development of a productive process. IP focuses on drastic performance developments rethinking the process as a whole and may even lead to the manufacture of new products that may not be produced by conventional process technologies " (Keil, 2007).

As can be seen from the above definitions, IP is a field of research under development and is still far from being classified as a mature art of development for processes and projects. In any case, there is a consensus that IP involves an integrated approach to various fields of research. In IP the journey is the reward. (Keil, 2007).

Considering that a universal definition of IP does not yet exist, for the development of this study, the definition proposed in the work of Lutze and Gorak will be used. "Process Intensification is defined as the improvement of a process through the targeted improvement of performance-limiting phenomena at different scales" (Lutze et al, 2013).

2.3 Stages of process intensification

According to Westerberg (2004) innovation in Process Intensification can be achieved when working on lower scales, that is, on the scale of phenomena. The method for the design and analysis of such a route followed by an additional study to generate other, more sustainable routes can be categorized into three main steps: (1) synthesis, (2) design and analysis, and (3) sustainable project (Kongpanna et al, 2014).

The purpose of the Design and Analysis step is to calculate the design variables, for example, equipment parameters. This makes it possible to describe the unit operations on the chosen processing route and its evaluation for the identification of process hot spots. A process hot-spot is a limiting / bottleneck in a process, which affects its performance and whether improved / eliminated increases overall process performance. In this way the objective of the Design and Analysis stage can also be transcribed as the improvement or elimination of a process hot-spot. The objective of the Sustainable Project stage is to generate more sustainable processing alternatives that have improvements in economic, sustainability and LCA factors. To assess whether a more sustainable project was achieved, different performance metrics can be plotted on a radar diagram, for example. Thus, the outer axis represents the base case design and any value within the diagram shows an improvement.

Synthesis / Intensification of processes can be defined, according to Babi et al. (2015) such as: generation of sustainable processes for the production of a specific product. These new process designs may include already existing hybrid / intensified units or new units capable of providing improvements in the efficient use of sustainability metrics and LCA factors, when compared to a base case. Thus, for the purposes of this study, the hybrid method proposed by Babi et al. (2015).

2.3.1 Application of IP / SP at different scales

Phase-based PI is defined as the generation of more sustainable projects by combining lower-level phenomena (PBBs) that perform a task on a larger scale (task). Therefore, in performing IP based on the phenomena scale, PBBs are combined to form simultaneous phenomena (SPBs), which in turn are combined to form basic structures that execute a task or set of tasks, using for this pre-defined rules. These basic structures are then translated into unit operations (higher scale) that constitute the final alternatives of flowcharts. The combination of PBBs to generate basic structures is a rule based and analogous to CAMD, proposed by Harper et al. (2000) where the atoms are combined to generate functional groups which in turn are combined to form molecules with a set of

desired properties (performance criteria). Babi et al. (2015) presents a comparative flowchart between these two phenomena-based syntheses.

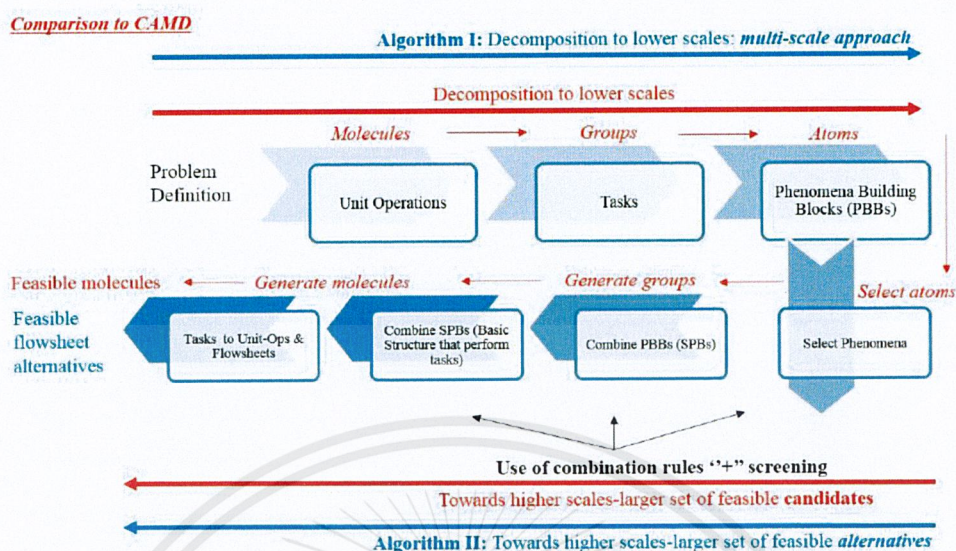


Figure 1: The concept of process synthesis-intensification framework compared to computer-aided molecular design (CAMD) (Babi et al., 2015).

A Phenomenon Building Block (PBB) is considered to be the smallest unit that performs a task in a process. For example, a mixing PBB performs a mixing task. A simultaneous phenomena building block (SPB) is defined as the combination of one or more building blocks of phenomena, using predefined combination rules. Most of the chemical processes can be represented by different combinations of mass transfer, energy and momentum phenomena (Lutze et al, 2013), such as mixing (M), two-phase mixing (2phM), heating (H), cooling (C), reaction (R), phase contact (PC), phase separation (PS), phase transition (PT) and divisor (D). The inlet / outlet flows of the PBBs are liquid (L), vapor (V), solid (S) and / or combinations thereof, for example, vapor and liquid (VL), liquid-liquid (LL), vapor- liquid (VLL) and solid-liquid (SL). (Babi et al, 2015). It should be noted that all possible combinations of SPBs are obtained from the combinations of the above 9 PBBs listed. The 9 building blocks of individual phenomena are used in the generation of SPBs using the

1. M - If separation or reaction occurs, mixing of the compounds before and / or after the reaction is necessary, thus an "M" PBB is required;
2. R - If a reaction occurs, the raw materials are converted into products, therefore an "R" PBB is required;
3. 2phM - If separation or reaction occurs in a two-phase system, the mixing of the two phases occurs, therefore a PBB "2phM" is required;
4. PC - If two phases are present, then the contact between the two phases occurs, therefore a PBB "PC" is required;
5. PT - If two phases are present, the transition from one phase to the other occurs. Thus, it is necessary to use a "PT" PBB;
6. PS - If two phases are present, the separation of these two phases occurs, therefore a PBB "PS" is required;
7. H / C - If one or more phases are present and there are changes in enthalpy due to internal and / or external energy sources, an "H" or "C" PBB is required;
8. D - If the division of flows is necessary, use of a PBB "D"

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2.4 Urea production process

In this paper, the production of urea through CO₂ stripping was considered as a base case design. Modeling and simulation were taken from previous work from (Chinda et al, 2017). Given that, this paper will provide just a general description of the process, the modelling and the simulation.

This process can be divided into five blocks: Synthesis, Evaporation, Desorption and Hydrolysis, Recirculation and Prilling, as it can be seen in Figure 2.

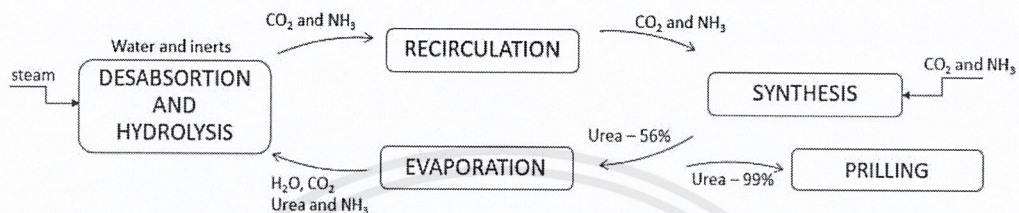
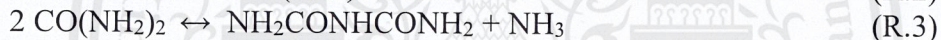


Figure 2: Simplified block diagram for the urea production process.
(Adapted from Chinda et al, 2017)

The three reactions occurring at this process and considered in this paper are the formation of ammonium carbamate (R.1), urea (R.2) and biuret (R.3).



The main reactions occurring in this process are the well know exothermic ammonium carbamate formation (R.1), the endothermic urea formation (R.2) and, finally, the endothermic biuret formation (R.3). Among these reactions, the biuret formation from two urea molecules is a highlight point in this study since there are few works concerning modelling and simulation and taking into account this reaction, as reported in (Chinda et al, 2017).

The main equipment in the Synthesis section are the pool condenser, the reactor, the scrubber and the stripper. This area of the process is responsible for the formation of ammonium carbamate and urea. After leaving the Synthesis section, the liquid product from the Stripper is forwarded to Recirculation. This section is responsible for removing the ammonium carbamate present in the solution through its decomposition in NH₃ and CO₂, besides to condense this same NH₃ and CO₂ again into carbamate that will be sent to the Synthesis section. The Recirculation section consists of the rectifying column and its respective heaters, condensers and an atmospheric flash tank. The product of this section goes to Evaporation section in order to concentrate the urea solution from the flash tank from 70% up to 99.5% to be pearled in the Prilling Tower. This section operates under vacuum, so that most of the water, ammonia, and carbon dioxide are removed from the solution. The Evaporation Section consists mainly of three evaporators and its respective heaters. The product of this section also goes to the Prilling tower. The last section is Desorption and Hydrolysis consisting of an adsorber and two desorber units. The main function of this section is to recovery NH₃, CO₂ and urea present in the water that comes from the Evaporation section.

Chapter III

Research Methodology

As shown in Figure 3, the overview of the framework inspiration from the paper by Babi et al. (2015) consists of two-parts involving base case design analysis-part and sustainable design-part or innovation-part that are briefly discussed below.

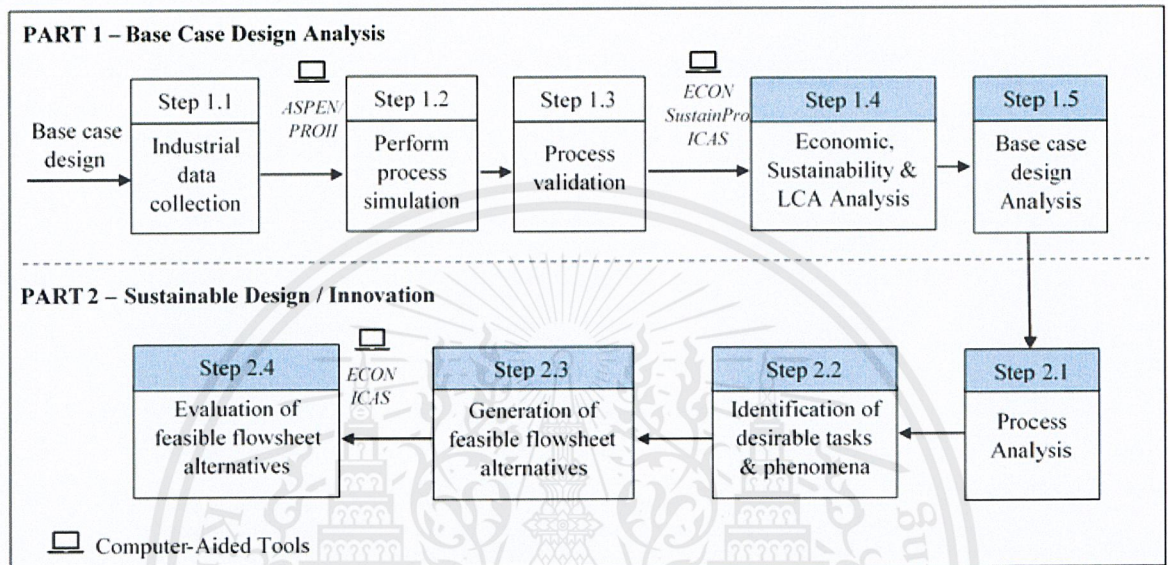


Figure 3: The overall framework for base case design process analysis and process intensification inspiration from the paper by Babi et al. (2015).

3.1 Part 1: Base case design analysis

Step 1.1. Industrial data collection

In this step all the industrial data as the main flows, composition, temperature and pressure along the entire process is collected. The intention in this step is to have enough information to model the process and also begin to collect data for validation of simulation. Factories usually have their own agenda for collecting data concerning stream compositions, as it can depend on laboratory schedule. The purpose here is to make a data collection without disturbances in daily operational routines. As it can take a lot of time, it is proposed to be the first step.

Step 1.2. Perform process simulation

The objective here is to perform a rigorous process simulation of the base case design. In principle, any process simulator could be used. However, before a rigorous simulation can be performed, it is important to check if all the necessary data are available. The appropriate unit operation models together with the consistent thermodynamic models will need to be employed from the selected simulator.

Step 1.3. Process validation

The main objective here is to perform the validation of the process using all the data collected in step 1.1. For this, firstly, a statistical analysis is required to treat all the industrial data in order to evaluate which ones can be used to validate the simulation. After this, the validation, properly saying, can properly be performed.

Step 1.4. Economic, Sustainability & LCA Analysis

In this step the base case design is analyzed using a sustainability, economic and LCA analysis. The sustainability analysis uses an indicator-based methodology where a set of calculated open paths (OPs) and closed paths (CPs) indicators are used to identify the structural bottlenecks. Through an open-path, mass (of a compound) and energy (carried by a compound) come in and go out of the system (process), while in a closed-path, they go around in cycles without going out (they represent recycle streams). The indicators therefore indicate whether a material or its energy equivalent loose value as they leave a process or if a large amount go around in cycles without going out. Through the values obtained for the indicators, it is possible to identify the location within the process where the mass/energy “path” faces “barriers” with respect to costs, benefits and accumulation. The sustainability analysis method can be found in a series of articles published by (Carvalho et al., 2008), (Carvalho et al., 2009) and (Carvalho et al., 2013).

Sustainability indicators:

1. Material value added (MVA): This indicator gives the value added between the entrance and the exit of a given compound, that is, the value generated or lost between the start and the end point of an open-path. Negative values of this indicator show that the compound has lost its value in this open-path and therefore point to a potential for improvement.

2. Energy and waste cost (EWC): This indicator is applied to both open- and closed-paths. It takes into account the energy costs (EC) and the costs related with the compound treatment (WC). The value of EWC represents the maximum theoretical amount of energy that can be saved in each path within the process. High values of this indicator show high consumption of energy and waste costs and therefore these paths should be considered in order to reduce the indicator value.

3. Total value added (TVA): This indicator describes the economic influence of a compound in a given path and is the difference between MVA and EWC. Negative values of this indicator show high potential for improvements in terms of decrease in the variable costs.

4. Accumulation factor (AF): This indicator determines the accumulative behavior of the compounds in the closed-paths. This corresponds to the amount that is recycled relative to the input to the process and not the inventory. High values of this indicator show high potentials for improvements.

Economic and Lifecycle Assessment (LCA) analysis, the economic evaluation provides an estimate of the operational cost and the LCA provides the environmental impact, for example, the carbon footprint and global warming potential.

Tools: For Sustainability analysis: The tools used for Sustainability analysis are fully described in (Carvalho et al., 2008) and (Carvalho et al., 2009) and its corresponding software-tool, SustainPro (Carvalho et al., 2013). For the economic evaluation: ECON (Saengwirun et al., 2011), a software for cost calculation and economic analysis. For the LCA: Using UK Government GHG conversion factors (Strategy, 2018) factors to calculate the carbon footprint of a process. And using the software Integrated Computer Aided System (ICAS) (Tallis, 2002) to generate the Waste Reduction (WAR) algorithm results.

Step 1.5. Base case design Analysis

The objective in this step is to identify the potential bottlenecks (process hot-spots) of base case design through a more detailed and rigorous simulation and indicator based analysis. And then targets for overcoming these “hot-spots” are defined in terms of process efficiency, productivity and sustainability as well as reduced energy consumption, waste generation, and environmental impact. The target indicator with a target value for improvement can be achieved through minimum changes in one or more operational variables related to the indicator.

3.2 Part 2: Sustainable design or innovation

The objective here is to generate and evaluate process alternatives that match the established targets for process improvements. More details of the process intensification based method employed here can be found in Babi et al. (2015). The method operates at the phenomena level and the concept is similar to that of computer-aided molecular design (CAMD), as show in Figure 1, where groups of atoms are used as building blocks to generate new as well as known molecules with desired (target) properties.

Step 2.1. Process Analysis

In this step, the base case design is analyzed in order to further identify/classify the process bottlenecks through a knowledge-based and a model-based approach. All mass and energy data are collected from the rigorous simulation of the base case design and the flowsheet is transformed into a task and phenomena based flowsheet in order to decouple the analysis from physical unit operations. The identified process bottlenecks are subsequently linked to corresponding phenomena and tasks inside and outside of the unit operation in which they occur. For analyzing the properties of the pure compounds in the system used the software Integrated Computer Aided System (ICAS). The binary ratio matrix (Jaksland et al., 1995) is calculated as the ratio between pure compound properties for all binary pairs formed by the mixture compounds. The number of binary pairs, NB, is given by $NB = NC(NC - 1)/2$, where NC is the number of compounds in the mixture. The binary ratio, r_{ij} , for a binary pair is calculated as, $r_{ij} = p_{A_j}/p_{B_j}$, where p is the pure component property.

Step 2.2. Identification of desirable tasks & phenomena

In this step additional phenomena for synthesis of flowsheets, which match the targets defined in Step 1.3 and thereby improve the process performance of the necessary phenomena (identified in Step 2.1) are selected. That is, the identified process bottlenecks and the corresponding phenomena and tasks are used to identify tasks and phenomena that need to be improved to achieve the desired performance. For the selection of suitable (desirable) phenomena, property analysis of single compound and mixtures of compounds

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as well as reactions in the system are needed. From the set of suitable phenomena the most promising phenomena are selected. However, some phenomena cannot be used on their own; hence, additional accompanying phenomena are selected. Finally, the operating window of all identified phenomena in the search space is determined. These are needed as input for the next step.

Step 2.3. Generation of feasible flowsheet alternatives

In this step all phenomena based process options are generated. The input to this step is the initial search space of identified phenomena and its corresponding operating windows. Next, all phenomena are connected to form feasible simultaneous phenomena building blocks (SPBs). By combining the phenomena in different ways (using combination rules), the same and new (combined) tasks can be performed, thereby leading to new and more sustainable alternatives that match the design targets.

Step 2.4. Evaluation of feasible flowsheet alternatives

After the process alternatives are generated in step 2.3, they are analyzed in terms of sustainability, economic and LCA evaluations. The objective of this step is to evaluate the alternatives to identify the best (or a sub-set) process. The performance evaluation of process alternatives are established in terms of carbon footprint (CF), which is the overall amount of carbon dioxide and other greenhouse gas emissions associated with 1 kg of product, the global warming potential (GWP) in terms of kg of CO₂ equivalent. For the health issues, an indicator such as the Human Toxicity Potential by Ingestion (HTPI) is used in terms of one per lethal concentration. Economic evaluation is calculated using ECON (Saengwirun, 2011) which provides the needed cost.

Chapter IV

Results and Discussion

4.1 Case study

The base case studied in this paper is the production of urea through CO₂ stripping. This process can be divided in five blocks: Synthesis, Evaporation, Desorption and Hydrolysis, Recirculation and Prilling. Description of the urea production process explain briefly in previous topic, 2.4 urea production process.

4.2 Part 1: Base case design analysis

Step 1.1. – 1.3. Industrial data collection, Perform process simulation and Process validation

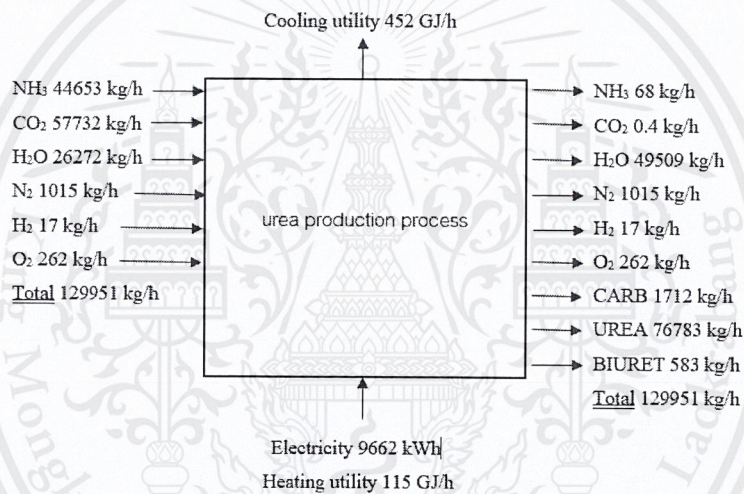


Figure 4: Calculated mass (kg/h) and energy (GJ/h) balance for the base case design of urea production process.

The experimental data used for validating the simulation was provided by an industrial urea plant. Simulation of urea production (Synthesis, Evaporation, Hydrolysis and Desorption and Recirculation part) is performed using the Aspen Plus process simulator. This process was modelled assuming steady state conditions, SR-POLAR for thermodynamic representation, production of biuret in the Pool Condenser, Reactor, Stripper and in all the Evaporators. Kinetics models were taken from (Chinda et al, 2017). Ammonia containing 2.24 wt.% of nitrogen, oxygen, hydrogen and water and carbon dioxide containing 0.2 wt.% of water are used as feedstock for detailed simulation of urea production process. The mass and energy balance are simply depicted in Figure 4.

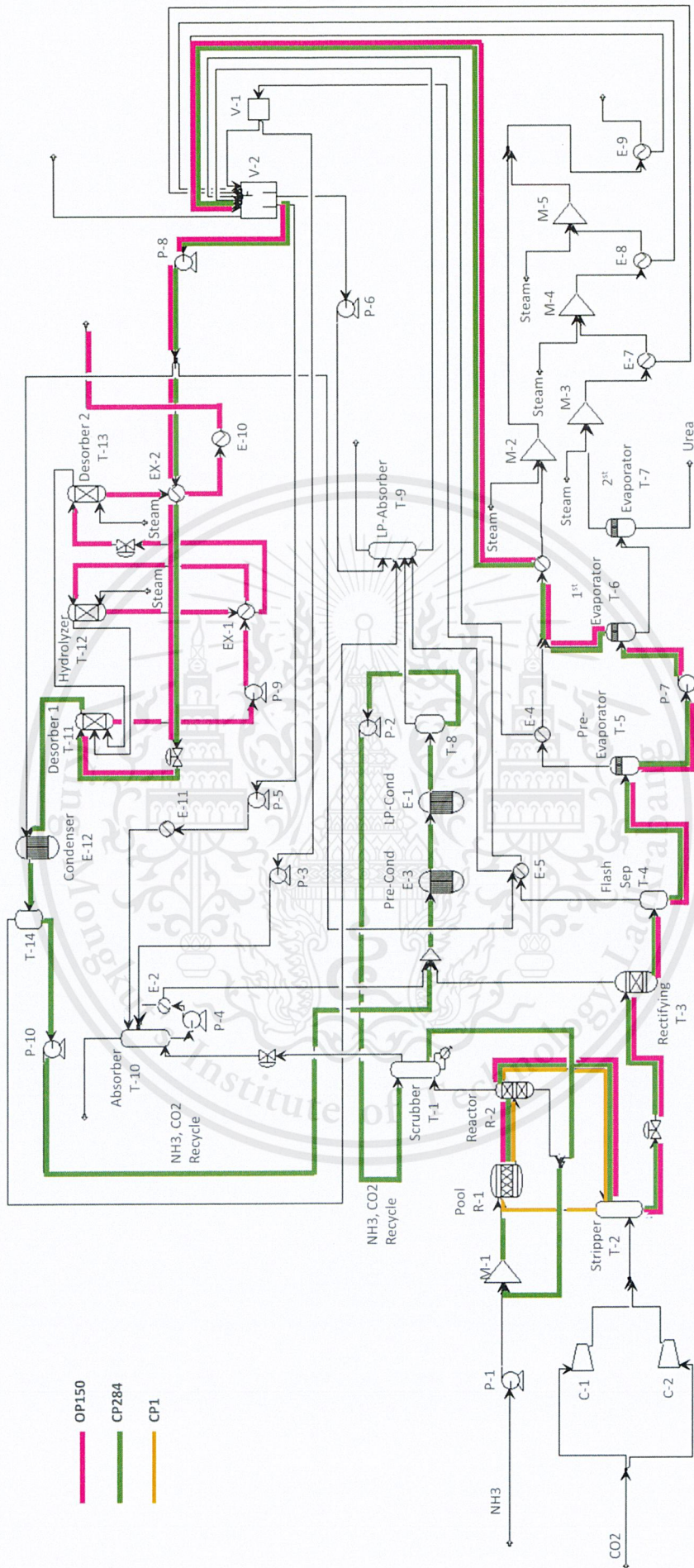


Figure 5: Base case simulation for the production of urea consists of four parts: Synthesis, Evaporation, Hydrolysis and Desorption and Recirculation. Including process bottlenecks, closed- and open-paths.

In process validation step, a statistical analysis based on dispersion was performed with the plant capacity in order to exclude data that may have been taken in transient process conditions. For this it was considered that coefficient of variation less than 1.5 % would reflect stability in operation of the industrial plant. A total of 37 different process parameters were evaluated following these criteria, among them stream temperature, steam generation, mass fraction composition for CO₂, NH₃, urea, H₂O and biuret, CO₂ conversion in the reactor and stripper efficiency. For all mass fractions evaluated, the deviation between the value predicted by the simulation and the real value obtained from industrial data were less than 5%, while for steam generation and streams temperature the deviation was less 8%. In this paper, not show details of process validation.

Step 1.4. Economic, Sustainability & LCA Analysis

The sustainability indicators on the more detailed base case calculations are given in Table 1 and the paths with which they are associated are given in Figure 5.

Table 1. The 4 most critical paths in the base case design that have the highest potentials for improvement. Note: OP-open path, CP-closed path.

Path	Compound	Flowrate (kg/h)	MVA (10 ³ \$/year)	TVA (10 ³ \$/year)	EWC (10 ³ \$/year)	AF (10 ³ \$/year)
OP150	H ₂ O	13471.370	-11	-177.204	166.427	-
CP284	H ₂ O	3438.333	-	-	47.220	0.030
CP1	NH ₃	23161.300	-	-	36.148	0.295

It can be seen in the Table 1, that water in the OP150 has a very negative value in terms of MVA and TVA indicators and very positive value in terms of EWC indicator, this means that water is losing its value as it exits the process through this path.

The CP284 which follows the path of water, has a high EWC. This means that a high flow of water is being recycled resulting in high loads of energy and waste/use of utilities for raw material recovery. The same also applies to ammonia in CP1. Thus, this path is identified as the one that contains the unit operations with potential bottlenecks. Table 2 gives a selected list of sustainability metrics for the base case design.

Table 2. Sustainability metrics for the base case design.

MJ energy/kg product	Kg product/kg raw material	Total kg CO ₂ Equivalent	Total utility costs (\$)/year
2.18	0.75	0.20	13,438,577.55

The economic and life cycle assessment analysis were also updated for the more detailed base case calculations and these are highlighted in Figure 6. In the urea production process, heating, cooling and electricity are the main drivers for operating cost. Utilities for heating/cooling are steam and cooling water, respectively. These are used by pump, compressor, reactor, heat exchangers, reboilers, and condensers that are present in the flowsheet. From Figure 6 it can be seen that columns T-3 (rectifying column), T-5 (pre-evaporator) and T-6 (1st evaporator), and compressors C-1 and C-2 have the large utility

cost in the process and therefore these are stored as process bottlenecks (high energy consumption) with respect to utility costs. And in Figures 6, it can be seen that same columns and same compressors and reactor R-1 (pool condenser) and heat exchanger E-6 have the large carbon footprint because of their high utility (energy) consumption.

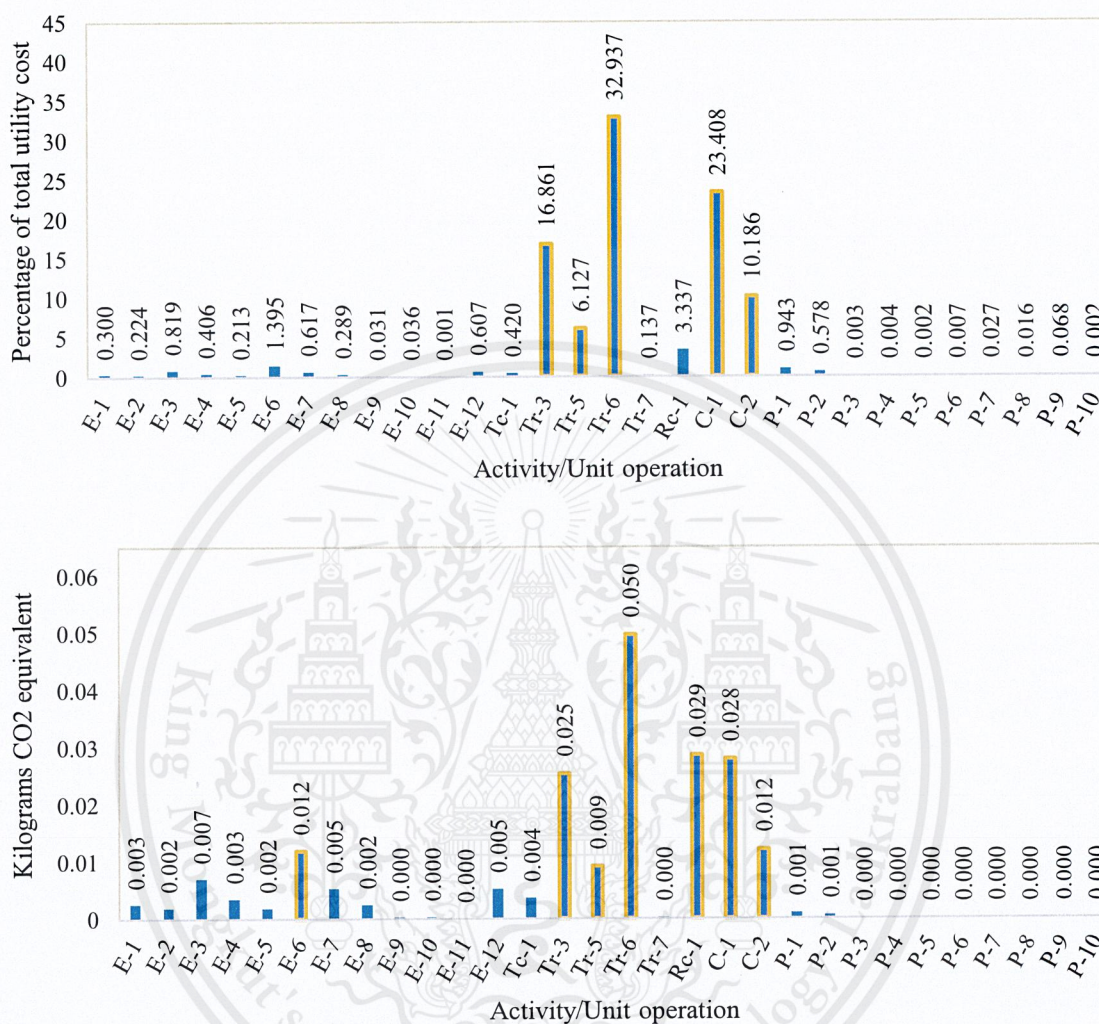


Figure 6: Economic analysis and LCA analysis for the base case design. Utility cost and Carbon footprint are compared.

Step 1.5. Base case design Analysis

The characteristics of the unit operations, for example, the above energy consumption analysis was stored as the final set of process bottlenecks. This information is useful because if these process bottlenecks are improved/eliminated then the new process alternative will be more sustainable and offer more economic benefits. Note that removing these bottlenecks means improvements in the corresponding indicators (from sustainability analysis), which in turns means improvement in the sustainability metrics. Thereby, a more sustainable process design is obtained. A list of the equipment according to their identification as a major bottleneck in the three (sustainability, cost, LCA) analyses is given in Table 3. It can be seen that columns T-3 (rectifying column), T-5 (pre-evaporator) and T-6 (1st evaporator) in the recirculation and evaporation part have appeared as a bottleneck in all three analyses. Therefore, from this analysis it can be concluded that the major

bottleneck of the process is very high energy consumption, which can be overcome by reducing the utility consumption and consequently utility costs.

Table 3. Main identified bottlenecks with respect to sustainability, economic and life cycle assessment (LCA) analysis.

Unit	Label	Sustainability	LCA	Economic
Reactor	R-1	X	X	
Reactor	R-2	X		
Column	T-1	X		
Column	T-2	X		
Column	T-3	X	X	X
Column	T-5	X	X	X
Column	T-6	X	X	X
Heat Exchanger	E-6	X	X	
Compressor	C-1		X	X
Compressor	C-2		X	X

Table 4. Identified process hot-spots for the base case design.

Indicator values	Base case property	Cause	Identified process hot-spot
α_2 = Utility cost β_1 = MVA β_2 = EWC γ_1 = CO2 equivalent γ_2 = PEI	products recovery	High energy usage heating and/or cooling	High energy consumption and/or demand

Note: Economic (α), sustainability (β) and LCA (γ) analysis, MVA – mass value added, EWC – Energy to waste cost, CO2 equivalent – carbon footprint, PEI – potential, environmental impact.

The design targets to be set/met are:

1. Reduce energy consumption
2. Reduce utility cost
3. Improvements in LCA/Sustainability indicators
4. Unit operations reduction
5. Product purity (kept as the base case)
6. Raw material (kept as the base case)

4.3 Part 2: Sustainable design or innovation

Step 2.1. Process Analysis

The base case design flowsheet was then transformed into a task based flowsheet, which identifies different tasks in the process in terms of mixing, reaction and/or separation tasks. The task based flowsheet of the base case design is shown in Figure 7. The phenomena based flowsheet of the base case design is generated and shown in Figure 8. The identified

phenomena building blocks (PBBs) are R (reaction), M (mixing), 2phM (two phase mixing), PC(VL), PT(VL), PS(VL), H (heating) and C (cooling) where, PC is phase contact; PT is phase transfer and PS is phase separation; while V, L and S represent vapor, liquid and solid phases.

The pure component and mixture property analysis is performed using ICAS. The binary ratio matrix analysis are presented in Table 5. From the boiling point binary ratio matrix value can pre-conceive that binary azeotrope is not found in this process because no binary pair that has a value close to unity.

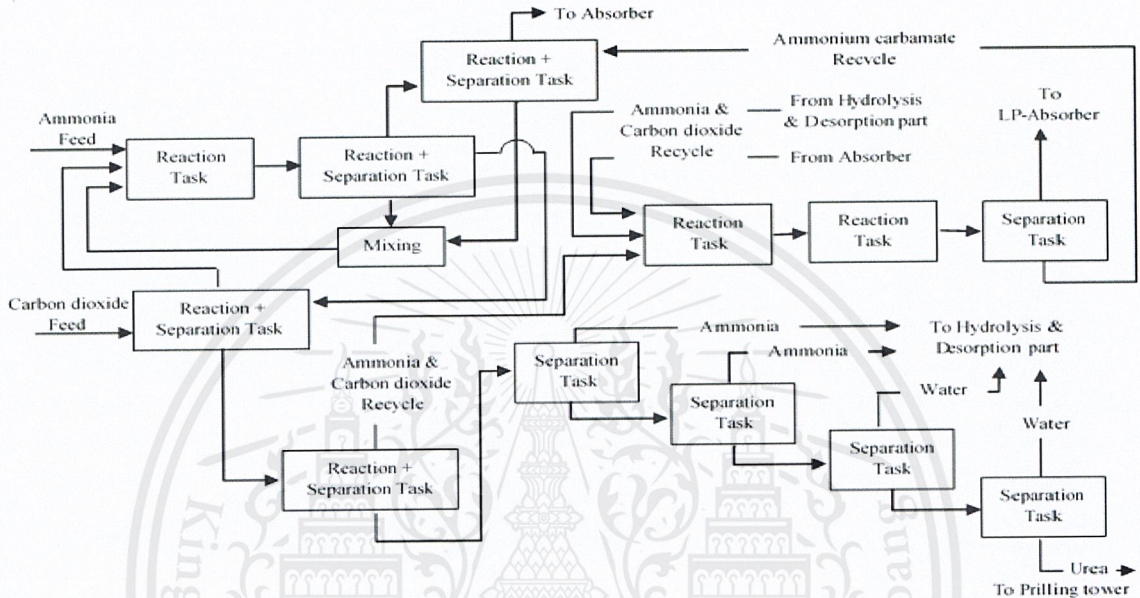


Figure 7: The task-based flowsheet of the base case design for urea production process.

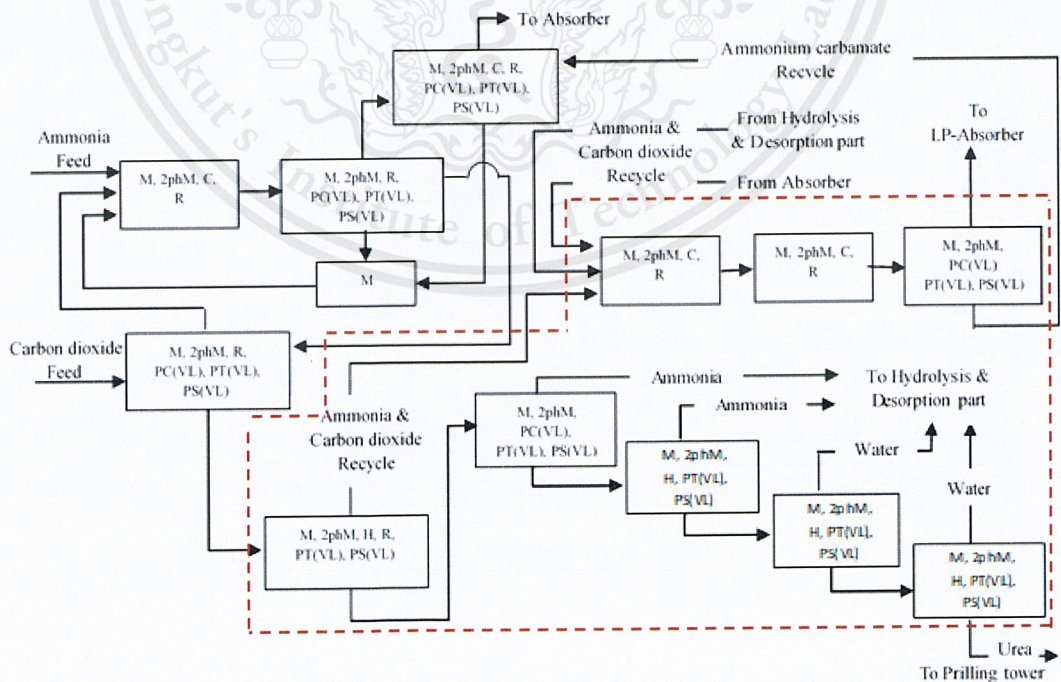


Figure 8: Phenomena based flowsheet of the base case design for urea production process.

Table 5. Binary ratio matrix for a set of selected properties.

rij (binary pair)	Property binary ratio							
	MW	Tm	Tb	SolPar	RG	VdW	VM	VP
NH3/CO2	2.58	1.11	1.29	2.01	1.22	1.43	1.49	NA
NH3/CARB	4.58	1.70	2.66	NA	NA	2.31	2.35	NA
NH3/UREA	3.53	2.08	1.94	1.24	3.05	2.34	1.95	NA
NH3/H2O	1.06	1.40	1.56	1.64	1.39	1.12	1.38	NA
NH3/N2	1.64	3.09	3.10	3.22	1.56	1.14	1.39	NA
NH3/H2	8.45	14.01	11.76	4.40	2.30	2.18	1.14	NA
NH3/O2	1.88	3.59	2.66	3.57	1.25	1.06	1.12	NA
NH3/BIURET	6.05	2.41	3.03	1.31	NA	3.30	6.27	NA
CO2/CARB	1.77	1.54	3.44	NA	NA	1.62	1.57	NA
CO2/UREA	1.36	1.87	2.51	2.49	2.50	1.64	1.31	NA
CO2/H2O	2.44	1.26	2.02	3.28	1.69	1.59	2.06	NA
CO2/N2	1.57	3.43	2.39	1.60	1.90	1.25	1.08	NA
CO2/H2	21.83	15.53	9.08	2.19	2.80	3.12	1.30	NA
CO2/O2	1.38	3.98	2.05	1.78	1.53	1.52	1.33	NA
CO2/BIURET	2.34	2.17	3.92	2.64	NA	2.31	4.20	NA
CARB/UREA	1.30	1.22	1.37	NA	NA	1.01	1.20	167.80
CARB/H2O	4.33	1.22	1.71	NA	NA	2.58	3.25	1929524.86
CARB/N2	2.79	5.27	8.23	NA	NA	2.02	1.69	NA
CARB/H2	38.73	23.87	31.23	NA	NA	5.05	2.05	NA
CARB/O2	2.44	6.13	7.06	NA	NA	2.46	2.09	NA
CARB/BIURET	1.32	1.41	1.14	NA	NA	1.43	2.67	4.91
UREA/H2O	3.33	1.49	1.25	1.32	4.23	2.61	2.70	11498.87
UREA/N2	2.14	6.43	6.01	3.99	4.75	2.05	1.41	NA
UREA/H2	29.79	29.09	22.81	5.45	7.01	5.12	1.71	NA
UREA/O2	1.88	7.47	5.16	4.43	3.82	2.49	1.74	NA
UREA/BIURET	1.72	1.16	1.56	1.06	NA	1.41	3.21	823.54
H2O/N2	1.56	4.33	4.82	5.26	1.12	1.28	1.92	NA
H2O/H2	8.94	19.58	18.30	7.19	1.66	1.96	1.58	NA
H2O/O2	1.78	5.02	4.14	5.84	1.11	1.05	1.55	NA
H2O/BIURET	5.72	1.72	1.94	1.24	NA	3.68	8.67	9469834.09
N2/H2	13.90	4.53	3.79	1.37	1.47	2.50	1.21	NA
N2/O2	1.14	1.16	1.17	1.11	1.24	1.22	1.24	NA
N2/BIURET	3.68	7.45	9.38	4.23	NA	2.88	4.52	NA
H2/O2	15.87	3.90	4.42	1.23	1.83	2.06	1.02	NA
H2/BIURET	51.13	33.74	35.58	5.78	NA	7.21	5.48	NA
O2/BIURET	3.22	8.66	8.04	4.70	NA	3.51	5.59	NA

MW – molecular weight (g/mol), Tb – normal boiling point (K), RG – radius of gyration (Å), Tm – normal melting point (K), VM – molar volume (m³/kmol), SolPar – solubility parameter, VDW – Van der Waal volume (m³/kmol), VP – vapor pressure (atm), NA – not available.

Step 2.2. Identification of desirable tasks & phenomena

According to Babi et al. (2015), the process hot-spots can be reduced/eliminated through the use of additional, desirable PBBs using thermodynamic insights. Each process hot-spot is linked to a binary ratio property (Jakslund et al., 1995) that translates into a (desirable) PBBs (see examples in Table 6.). For example, if the molar volume binary ratio is greater than 1.5 (Jakslund et al., 1995) then the PBB PT(PVL) is selected and added to the initial set of PBBs. This PBB is the building block of a pervaporation membrane or unit operation that incorporates pervaporation at the unit operations scale. Considering phenomena at process bottleneck area, evaporation and recirculation section, (red dotted box in Figure 8.), the reaction in rectifying column is a decomposition reaction of carbamate that are left from the synthesis part. From Table 5, it can be seen that for the UREA/H₂O binary pair, the molar volume is 2.7 then the PBB PT(PVL) is selected. For the NH₃/H₂O binary pair, the solubility parameter is 1.64, the radius of gyration is 1.39 and molar volume is 1.38. Therefore, the PBBs PT(PVL), PT(VV) and PS(VV) are selected. In total 15 phenomena building blocks are identified: four mixing (ideal liquid, flow, rectangular, ideal vapor), 2phM, H, C, R, PT(VL), PT(PVL), PT(VV), PC(VL), PS(VL), PS(VV) and dividing (D).

Table 6. List of selected (desirable) PBBs linked to the identified tasks V – vapor, L – liquid, LL – liquid–liquid, MSA – mass separating agent (Babi et al., 2015).

Process-Hotspot	Main Task	Property/Binary Ratio	Alternative Task	MSA	PBB (desirable)
High energy consumption/demand	Separation	Vapor pressure, heat of-vaporization, boiling point, solubility parameter	Separation	Yes	PC(VL), PT(VL), PS(VL)
	Separation	Vapor pressure, heat of-vaporization, boiling point	Separation	No	PC(VL), PT(VL), PS(VL)
	Separation	Molar volume, solubility parameter, molar volume, radius of gyration, dipole moment	Separation	No	PT(PVL), PT(VV), PS(VV)

Step 2.3. Generation of feasible flowsheet alternatives

The maximum number of phenomena that can be combined to form simultaneous phenomena building blocks (SPBs), by using predefined combination rules (Babi et al., 2015), $n_{PBB,Max}$, is calculated to be 11 (Equation 1). The total number of possible SPBs that can be generated, having a maximum of 11 PBBs is calculated to be 16278 (Equation 2). In Equation 1, $n_{PBB,max}$ is the maximum number of phenomena that can be present in an SPB, n_{PBB} is the total number of phenomena building blocks, 15, n_{PBB_E} is the total number of energy transfer phenomena, 2, n_{PBB_M} is the total number of mixing phenomena, 3, and n_{PBB_D} is the dividing phenomena, 1. In Equation 2 $NSPB_{Max}$ is the total number of possible SPBs.

$$n_{PBB,Max} = n_{PBB} - (n_{PBB_E} - 1) - (n_{PBB_M} - 1) - n_{PBB_D} = 11 \quad (\text{Equation 1})$$

$$NSPB_{Max} = \sum_{k=1}^{n_{PBB,Max}} \left(\frac{(n_{PBB}-1)!}{(n_{PBB}-k-1)!k!} \right) + 1 = 16278 \quad (\text{Equation 2})$$

However, not all combinations are feasible. The combination rules proposed by Babi et al. (2015) for example, SPBs containing the combination of H and C PBBs to form =H=C=

are rejected because of thermodynamic infeasibility, using these rules 70 SPBs are found to be feasible. A list of feasible SPBs assuming three types of mixing (idea, tubular flow, rectangular flow) are presented in Table 7.

Table 7. Partial list of feasible SPBs. Mix. – mixing, Cool. – cooling, Heat. – heating, React. – reaction, Sep. – separation, Ph. Cr. – phase creation, Div. – dividing.

SPB	Connected PBB	In	Out	Task they may perform
SPB.1	M	1..n(L,VL,V)	1(L,VL,V)	Mix.
SPB.2	M=2phM	1..n(L,VL,V)	1(L,VL,V)	Mix.
SPB.3	M=R	1..n(L,VL,V)	1(L,VL,V)	Mix.+ React.
SPB.4	M=H	1..n(L,VL,V)	1(L,VL,V)	Mix.+ Heat.
SPB.5	M=C	1..n(L,VL,V)	1(L,VL,V)	Mix.+ Cool.
SPB.6	M=R=H	1..n(L,VL,V)	1(L,VL,V)	React.+ Heat.
SPB.7	M=R=C	1..n(L,VL,V)	1(L,VL,V)	React.+ Cool.
SPB.8	M=R=H=PC(VL)=PT(VL)	1..n(L,VL,V)	1(L,VL,V)	React.+ Heat.
SPB.9	M=R=C=PC(VL)=PT(VL)	1..n(L,VL,V)	1(L,VL,V)	React.+ Cool.
SPB.10	M=R=2phM=PC(VL)=PT(VL)	1..n(L,VL)	2(V/L)	React.+ Sep.
SPB.11	M=R=2phM=PC(VL)=PT(VL)=PS(VL)	1..n(L,VL)	2(V;L)	React.+ Sep.
SPB.12	M=R=2phM=PC(VL)=PT(PVL)=PS(VL)	1..n(L,VL)	2(V;L)	React.+ Sep.
SPB.13	M=R=H=2phM=PC(VL)=PT(PVL)=PS(VL)	1..n(L,VL)	2(V;L)	React.+ Sep.
SPB.14	M=R=C=2phM=PC(VL)=PT(PVL)=PS(VL)	1..n(L,VL)	2(V;L)	React.+ Sep.
SPB.15	M=2phM=PC(VL)=PT(VL)	1..n(L,VL)	2(V;L)	Mix.+ Ph. Cr
SPB.16	M=2phM=C=PC(VL)=PT(VL)	1..n(L,VL)	2(V;L)	Mix.+ Ph. Cr.
SPB.17	M=2phM=H=PC(VL)=PT(VL)	1..n(L,VL)	2(V;L)	Mix.+ Ph. Cr.
SPB.18	M=2phM=PC(VL)=PT(VL)=PS(VL)	1..n(L,VL)	2(V;L)	Mix.+ Sep.
SPB.19	M=C=2phM=PC(VL)=PT(VL)=PS(VL)	1..n(L,VL)	2(V;L)	Cool.+ Sep.
SPB.20	M=H=2phM=PC(VL)=PT(VL)=PS(VL)	1..n(VL)	2(V;L)	Heat.+ Sep.
SPB.21	M=2phM=PC(VL)=PT(PVL)=PS(VL)	1..n(VL)	2(V;L)	Mix.+ Sep.
SPB.22	M=2phM=PC(VL)=PT(VV)=PS(VV)	1..n(L,VL,V)	2(V;V)	Mix.+ Sep.
SPB.23	M=2phM=PT(VV)=PS(VV)	1..n(V)	2(V;V)	Mix.+ Sep.
SPB...
SPB.70	D	1(L;VL,V)	1..n(L;V;VL)	Stream Div.

Note: V = vapor, L = liquid, “/” means “or”, “;” means “and”, “In” provides number of inlet streams (1 to n) and phase, “Out” provides number of outlet streams (1 or 2) and phase.

The identified feasible SPBs are combined to form basic structures. These basic structures are formed in a way that they satisfy the identified reaction and/or separation tasks. These combinations of basic structures are then translated to unit-ops, as show in Table 8. Two intensified flowsheet alternatives are generated, as shown in Figure 9.

Table 8. Generation of hybrid/intensified unit operations from combination of PBBs. Considering at evaporation and recirculation section.

SPB	Combined SPBs (basic structure)	Task Performed	Unit operations
SPB.6	$M(VL)=R(VL)=H$		Conventional Reactor
SPB.2 SPB.4 SPB.21	$M(VL)=2phM$ $M(L)=2phM=PC(VL)=PT(PVL)=PS(VL)$ $M(L)=H$		Pervaporation membrane unit
SPB.23	$M(V)=2phM=PT(VV)=PS(VV)$		Vapor permeation membrane unit
SPB.18 SPB.19 SPB.20	$M(VL)=C=2phM=PC(VL)=PT(VL)=PS(VL)$ $M(VL)=2phM=PC(VL)=PT(VL)=PS(VL)$ $M(VL)=H=2phM=PC(VL)=PT(VL)=PS(VL)$		Conventional distillation column
SPB.11 SPB.19 SPB.20	<div style="border: 1px dashed black; padding: 5px;"> $M(VL)=R(VL)=H$ $M(VL)=C=2phM=PC(VL)=PT(VL)=PS(VL)$ $M(VL)=2phM=PC(VL)=PT(VL)=PS(VL)$ $M(VL)=H=2phM=PC(VL)=PT(VL)=PS(VL)$ </div> <p style="text-align: center;">↓</p> <div style="border: 1px solid black; padding: 5px;"> $M(VL)=C=2phM=PC(VL)=PT(VL)=PS(VL)$ $M(VL)=R=2phM=PC(VL)=PT(VL)=PS(VL)$ $M(VL)=H=2phM=PC(VL)=PT(VL)=PS(VL)$ </div> <p style="text-align: center;">Basic structures are combined</p>	<div style="border: 1px dashed black; padding: 5px;"> </div> <p style="text-align: center;">↓</p>	Reactive distillation column

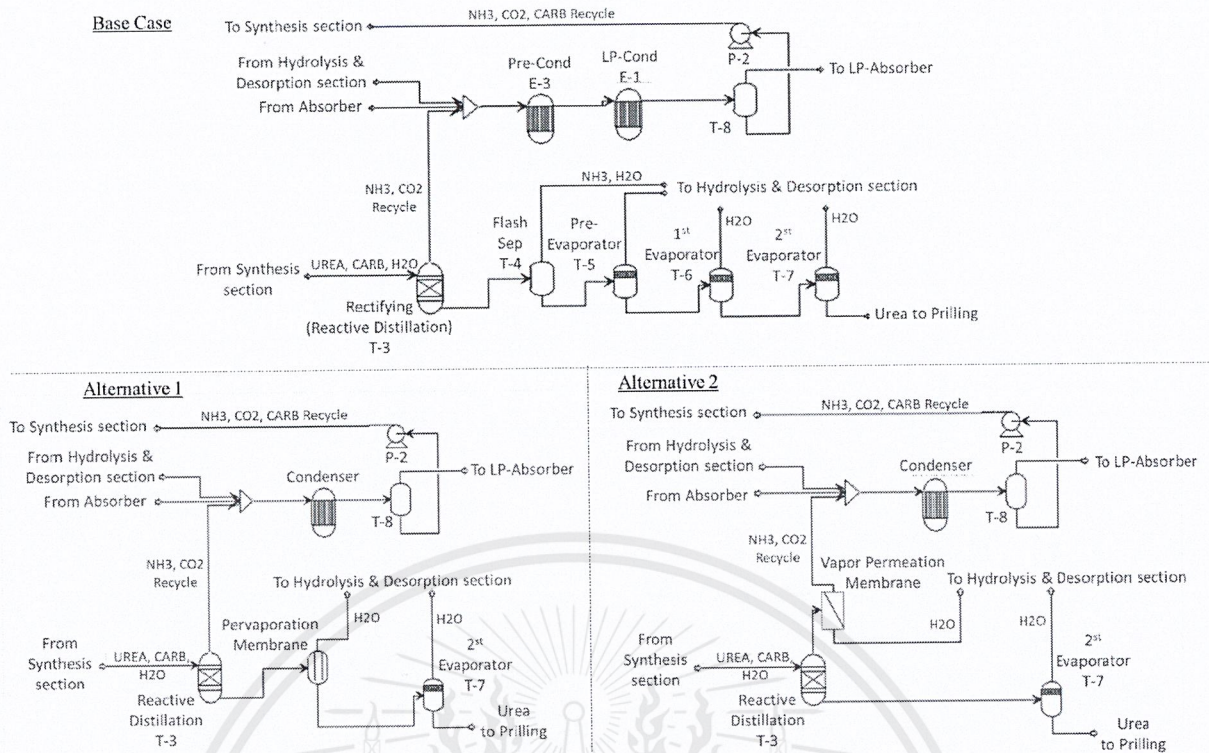


Figure 9: Base case and intensified flowsheet alternatives.

The following flowsheet alternatives are considered for the evaporation and recirculation section (red dotted box in Figure 8.).

- Flowsheet alternative 1 Pervaporation membrane unit for the separation of H₂O/Urea.
- Flowsheet alternative 2 Vapor permeation membrane unit for the separation of NH₃, CO₂/H₂O.

These flowsheet alternatives are generated using the following SPBs and further explained in Table 7:

- Pervaporation membrane: SPB. 21 M=2phM=PC(VL)=PT(PVL)=PS(VL).
- Vapor permeation membrane: SPB. 23 M=2phM=PT(VV)=PS(VV).
- Reactive distillation for reaction and separation: SPB. 11(M = R = 2phM = PC(VL) = PT(VL) = PS(VL)).

The generated flowsheet alternatives are shown in Figure 9. The rectifying column is like a reactive distillation column, it has both reaction, decomposition reaction of carbamate, and separation in this unit. In alternative 1, the integration of basic structures for the last three separation tasks is considered. This is possible as both separation tasks involve SPB involving separation of water from the urea in liquid phase. Thus, a basic structure having phenomena PT(VL), PT(PVL) and PS(VL) is selected. Additional PBBs like cooling, heating and mixing can also be added to the selected SPBs. Thus, in flowsheet alternative 1 the combined basic structure is translated to pervaporation membrane to obtain reduce energy consumption. In alternative 2, change condition of the reactive distillation column to separate water, ammonia and carbon dioxide from urea and then separate ammonia and carbon dioxide from water in another unit. Separation of ammonia and carbon dioxide from water in vapor phase, a basic structure having phenomena PT(VV) and PS(VV) is selected.

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Thus, in flowsheet alternative 2 the combined basic structure is translated to vapor permeation membrane.

In order to check feasibility of the proposed two intensified process alternatives for the production of urea they are first simulated with Aspen Plus. The steady state process simulation has been performed. Assumption for alternative 1, 90% of water can separate from urea in the pervaporation membrane. In alternative 2, the new conditions of reactive distillation are pressure 1 atm and temperature 404K, assumption for vapor permeation membrane is 90% of water can separate from ammonia and carbon-dioxide. The simulation results of the all process alternatives are used in the evaluation as well as the base case design in step 1.4.

Step 2.4. Evaluation of feasible flowsheet alternatives

Here, the performances of the generated alternatives are compared in terms of sustainability selected metrics, economic factors and life cycle assessment factors. The most important performance criteria for the base case and the intensified alternative are given in Table 9. The two process alternatives obviously offer superior performance in terms of all indicators to the base case process. The best process alternative is the pervaporation membrane option (alternative 1). The energy consumption per one unit of urea is significantly reduced (53.48%) as well as utility cost (42.27%). The hot utilities (steam/hot water) and cold utilities (cooling water) usage were reduced to 68.63% and 29.15%, respectively. In addition, the carbon footprint, HTPI and GWP were reduced to 41.63%, 1.51% and 1.39%, respectively. In this work, although only the evaporation and recirculation part have been targeted for intensification, it can be claimed that a more sustainable alternative has been achieved.

Table 9. Comparison of the base case design and the alternative design inclusive of process intensification.

	Sustainability Metrics	Base case design	alternative 1	alternative 2
Performance metrics	Total utility cost (\$/year)	13,438,578	7,893,752	11,951,072
	Total energy consumption (GJ/h)	149.352	70.687	131.124
	product/raw material (kg/kg)	0.75	0.76	0.76
	Energy/ products (MJ/kg)	1.9451	0.9048	1.6754
	Hot Utility (GJ/hr)	114.567	35.941	96.425
	Cold Utility (GJ/hr)	452.391	320.532	351.275
LCA	Total carbon footprint (kg CO ₂ eq.)	0.2014	0.1175	0.1665
	HTPI - Human Toxicity Potential by Ingestion (1/LD ₅₀)	4004.7	3389.39	3297.41
	GWP - Global Warming Potential (CO ₂ eq.)	0.30	0.04	0

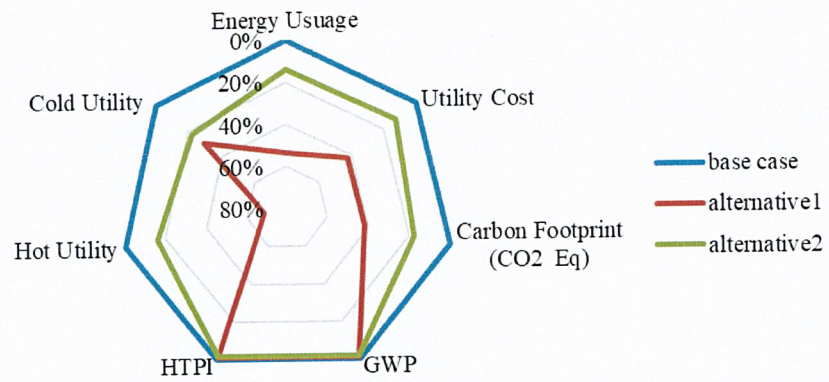


Figure 10: Process performance evaluation of the process alternatives compared to the base case design.



Chapter V

Conclusion

5.1 Summary

Hot-spots of urea production process were identified through economic, sustainability and LCA analysis. The major bottleneck occurred at evaporation and recirculation sections. The rectifying column, the pre-evaporator and the 1st evaporator have the large utility cost and also have the largest carbon footprint because of its high-energy consumption. By applying the phenomena based method, two feasible alternatives using pervaporation membrane and vapor permeation membrane were proposed. Alternatives 1 and 2 were simulated and evaluated economic and environmental factors. Compare base case and intensified flowsheets, the intensified alternatives are more sustainable in terms of the selected performance criteria.

5.2 Recommendations for further research

5.2.1 Next works should take into account studies to define the most suitable type of membrane to be employed in this case.

5.2.2 Used more indicators to analysis process for example capital cost in economic analysis to increase the chances of choosing the best process more precisely.

5.2.3 Expand the area to do intensification, not only evaporation and recirculation section, to generate more sustainable alternative process.

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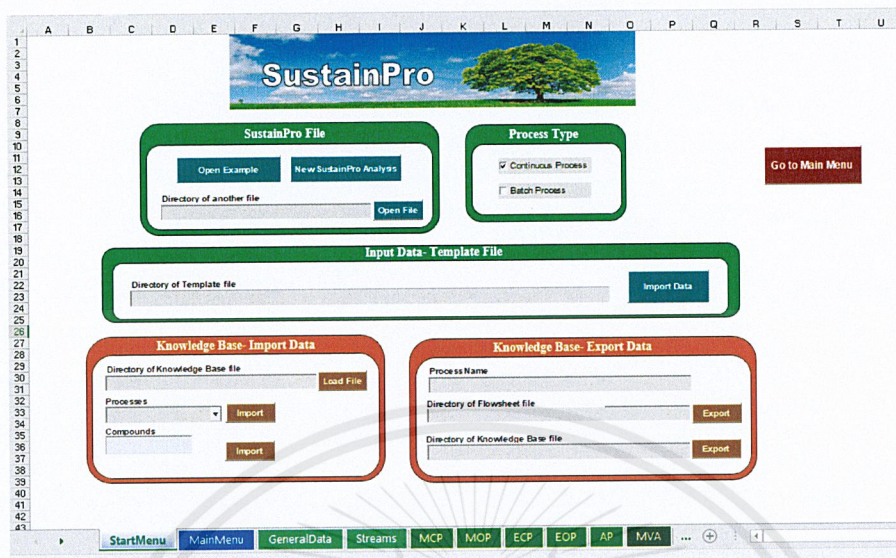
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A. Sustainability analysis of Base case design

SustainPro software



Utilities, raw material and product prices

Utilities	Price
Heating (HP) (\$/GJ)	9.83
Heating (MP) (\$/GJ)	8.22
Cooling (\$/GJ)	0.35
Electricity (\$/kWh)	0.06

Raw material price (\$/kg)	
CO ₂	0.03
NH ₃	0.5
H ₂ O	0.0008

Product price (\$/kg)	
Urea	0.35

Indicators summary results

Open Path	Component	Flowrate (kg/h)	MVA (103\$/yr)	EWC (103\$/yr)	TVA(103\$/yr)
OP 1	NH ₃	4609.739	Non Defined	9.6756	Non Defined
OP 2	NH ₃	2237.672	Non Defined	4.2981	Non Defined
OP 3	NH ₃	37091.230	Non Defined	24.4472	Non Defined
OP 4	NH ₃	2525.307	Non Defined	4.3912	Non Defined
OP 5	NH ₃	1225.841	Non Defined	1.9132	Non Defined
OP 6	NH ₃	20319.315	Non Defined	6.0765	Non Defined
OP 7	NH ₃	487.621	Non Defined	4.7583	Non Defined
OP 8	NH ₃	1784.933	Non Defined	17.0511	Non Defined
OP 9	NH ₃	0.484	-1	0.0138	-1.2090990
OP 10	NH ₃	41.688	-103	0.4521	-103.35540
OP 11	NH ₃	1909.495	Non Defined	18.63318518	Non Defined
OP 12	NH ₃	6989.690	Non Defined	66.77102387	Non Defined
OP 13	NH ₃	1.896	-5	0.054216223	-4.7347580
OP 14	NH ₃	163.246	-403	1.7702	-404.73344
OP 15	NH ₃	3.526	Non Defined	0.0057	Non Defined
OP 16	NH ₃	12.907	Non Defined	0.0182	Non Defined
OP 17	NH ₃	266.285	Non Defined	0.2400	Non Defined
OP 18	NH ₃	0.173	0	0.0000	-0.4270898
OP 19	NH ₃	0.339	Non Defined	0.0005	Non Defined

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Open Path	Component	Flowrate (kg/h)	MVA (103\$/yr)	EWC (103\$/yr)	TVA(103\$/yr)
OP 20	NH3	1.239	Non Defined	0.0017	Non Defined
OP 21	NH3	25.567	Non Defined	0.023039008	Non Defined
OP 22	NH3	9.348	-23.074	0	-23.075251
OP 23	NH3	18.291	Non Defined	0.030	Non Defined
OP 24	NH3	66.953	Non Defined	0.09	Non Defined
OP 25	NH3	1381.335	Non Defined	1.24	Non Defined
OP 26	CO2	0.119	0	0.00	-0.003721
OP 27	CO2	0.296	Non Defined	0.00	Non Defined
OP 28	CO2	1.082	Non Defined	0.00	Non Defined
OP 29	CO2	3751.755	Non Defined	2.287885115	Non Defined
OP 30	CO2	1991.853	Non Defined	1.081426426	Non Defined
OP 31	CO2	32910.577	Non Defined	8.84425	Non Defined
OP 32	CO2	0.220	Non Defined	0.00016	Non Defined
OP 33	CO2	337.097	Non Defined	0.23886	Non Defined
OP 34	CO2	1233.940	Non Defined	0.77851	Non Defined
OP 35	CO2	0.052	0	6.95294E-05	-0.0016191
OP 36	CO2	0.129	Non Defined	0.000196245	Non Defined
OP 37	CO2	0.471	Non Defined	0.000681785	Non Defined
OP 38	CO2	1632.513	Non Defined	0.995534725	Non Defined
OP 39	CO2	866.721	Non Defined	0.470564519	Non Defined
OP 40	CO2	14320.484	Non Defined	3.848428176	Non Defined
OP 41	CO2	0.096	Non Defined	6.78778E-05	Non Defined
OP 42	CO2	146.682	Non Defined	0.103936687	Non Defined
OP 43	CO2	536.928	Non Defined	0.34	Non Defined
OP 44	CO2	0.098	0	0.00	-0.0030559
OP 45	CO2	0.244	Non Defined	0.00	Non Defined
OP 46	CO2	0.895	Non Defined	0.00	Non Defined
OP 47	CO2	3101.759	Non Defined	1.24	Non Defined
OP 48	CO2	1646.762	Non Defined	1	Non Defined
OP 49	CO2	27208.782	Non Defined	2	Non Defined
OP 50	CO2	0.182	Non Defined	0	Non Defined
OP 51	CO2	278.695	Non Defined	0	Non Defined
OP 52	CO2	1020.159	Non Defined	0	Non Defined
OP 53	CO2	1.559	Non Defined	0.00	Non Defined
OP 54	CO2	2387.300	Non Defined	1.19	Non Defined
OP 55	CO2	8738.689	Non Defined	3.69	Non Defined
OP 56	CO2	0.211	Non Defined	0.00	Non Defined
OP 57	CO2	0.774	Non Defined	0.00	Non Defined
OP 58	CO2	0.011	0	0.00	-0.0003365
OP 59	CO2	0.069	Non Defined	0.00	Non Defined
OP 60	CO2	47.809	Non Defined	0.021874853	Non Defined
OP 61	CO2	256.684	Non Defined	0.117444174	Non Defined
OP 62	CO2	0.020	Non Defined	1.30807E-05	Non Defined
OP 63	CO2	0.075	Non Defined	4.20679E-05	Non Defined
OP 64	CO2	0.007	Non Defined	3.06566E-06	Non Defined
OP 65	CO2	4.625	Non Defined	0.00	Non Defined
OP 66	CO2	24.833	Non Defined	0.011361983	Non Defined
OP 67	CO2	1.328	Non Defined	0.00084951	Non Defined
OP 68	CO2	4.861	Non Defined	0.002732049	Non Defined

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Open Path	Component	Flowrate (kg/h)	MVA (103\$/yr)	EWC (103\$/yr)	TVA(103\$/yr)
OP 69	CO2	0.069	0	3.1768E-05	-0.0021147
OP 70	CO2	0.435	Non Defined	0.000199095	Non Defined
OP 71	CO2	300.381	Non Defined	0.137437429	Non Defined
OP 72	CO2	1612.722	Non Defined	0.737889547	Non Defined
OP 73	CARB	1044.332	0	7.190161935	-7.1901619
OP 74	CARB	12038.363	Non Defined	14.98953043	Non Defined
OP 75	CARB	35980.552	Non Defined	15.29285447	Non Defined
OP 76	CARB	20512.675	Non Defined	8.718525415	Non Defined
OP 77	CARB	225.961	0	1.566865008	-1.5668650
OP 78	CARB	2604.731	Non Defined	3.371631385	Non Defined
OP 79	CARB	7785.085	Non Defined	3.692542894	Non Defined
OP 80	CARB	4438.312	Non Defined	2.105135384	Non Defined
OP 81	CARB	307.217	0	2.22	-2.22127675
OP 82	CARB	3541.397	Non Defined	5.63	Non Defined
OP 83	CARB	10584.613	Non Defined	8.15	Non Defined
OP 84	CARB	6034.335	Non Defined	4.65	Non Defined
OP 85	CARB	83.928	0	0.60	-0.5989154
OP 86	CARB	967.465	Non Defined	1	Non Defined
OP 87	CARB	2891.583	Non Defined	2	Non Defined
OP 88	CARB	1648.504	Non Defined	1	Non Defined
OP 89	CARB	0.457	0	0	-0.0034346
OP 90	CARB	5.272	Non Defined	0.01	Non Defined
OP 91	CARB	15.756	Non Defined	0.02	Non Defined
OP 92	CARB	8.982	Non Defined	0.01	Non Defined
OP 93	CARB	52.360	Non Defined	0.00	Non Defined
OP 94	CARB	541.262	Non Defined	0.00	Non Defined
OP 95	CARB	0.082	0	0.00	-0.0006469
OP 96	CARB	0.947	Non Defined	0.00	Non Defined
OP 97	CARB	2.830	Non Defined	0.004005799	Non Defined
OP 98	CARB	1.613	Non Defined	0.002283724	Non Defined
OP 99	CARB	50.444	0	0.382552093	-0.3825520
OP 100	CARB	581.490	Non Defined	1.130323895	Non Defined
OP 101	CARB	1737.971	Non Defined	1.953	Non Defined
OP 102	CARB	990.825	Non Defined	1.113	Non Defined
OP 103	CARB	0.008	Non Defined	0.000	Non Defined
OP 104	CARB	0.023	Non Defined	0.000	Non Defined
OP 105	CARB	0.013	Non Defined	0.000	Non Defined
OP 106	CARB	0.076	Non Defined	0.000	Non Defined
OP 107	CARB	0.784	Non Defined	0.000	Non Defined
OP 108	UREA	46056.018	-16120	275.471	-16395.077
OP 109	UREA	0.033	Non Defined	0.000	Non Defined
OP 110	UREA	286.365	Non Defined	1.840	Non Defined
OP 111	UREA	0.005	Non Defined	0.000	Non Defined
OP 112	UREA	0.358	0	0.002	-0.1277337
OP 113	UREA	0.148	Non Defined	0.001	Non Defined
OP 114	UREA	1285.037	Non Defined	8.212	Non Defined
OP 115	UREA	0.023	Non Defined	0.000	Non Defined
OP 116	UREA	47.784	Non Defined	0.051	Non Defined
OP 117	UREA	171.870	Non Defined	0.060	Non Defined

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Open Path	Component	Flowrate (kg/h)	MVA (103\$/yr)	EWC (103\$/yr)	TVA(103\$/yr)
OP 118	UREA	30738.889	-10759	181.423	-10940.033
OP 119	UREA	0.022	Non Defined	0.000	Non Defined
OP 120	UREA	191.127	Non Defined	1.213	Non Defined
OP 121	UREA	0.239	0	0.002	-0.0852336
OP 122	UREA	0.099	Non Defined	0.001	Non Defined
OP 123	UREA	857.664	Non Defined	5.413	Non Defined
OP 124	UREA	0.016	Non Defined	0.000	Non Defined
OP 125	UREA	31.892	Non Defined	0.031	Non Defined
OP 126	UREA	114.710	Non Defined	0.031	Non Defined
OP 127	H2O	1.322	0	0.016	-0.0167192
OP 128	H2O	-3.191	Non Defined	-0.043	Non Defined
OP 129	H2O	83.769	0	1.061	-1.1278490
OP 130	H2O	1.637	Non Defined	0.021	Non Defined
OP 131	H2O	37.485	0	0.028	-0.0576626
OP 132	H2O	-9.833	Non Defined	-0.014	Non Defined
OP 133	H2O	258.118	0	0.197	-0.4031014
OP 134	H2O	5.045	Non Defined	0.004	Non Defined
OP 135	H2O	-377.327	Non Defined	-0.585	Non Defined
OP 136	H2O	9904.521	-8	8.771	-16.694574
OP 137	H2O	193.604	Non Defined	0.169	Non Defined
OP 138	H2O	-220.754	Non Defined	-0.315	Non Defined
OP 139	H2O	5794.617	-5	4.423	-9.0584092
OP 140	H2O	113.267	Non Defined	0.085	Non Defined
OP 141	H2O	39.859	0	0.029	-0.0613146
OP 142	H2O	-10.456	Non Defined	-0.015	Non Defined
OP 143	H2O	274.465	0	0.209	-0.4286312
OP 144	H2O	5.365	Non Defined	0.004	Non Defined
OP 145	H2O	8759.391	-7	0.105	-7.112807
OP 146	H2O	2116.416	-2	0.025	-1.7185741
OP 147	H2O	41.370	Non Defined	0.000	Non Defined
OP 148	H2O	212.676	0	2.453	-2.6228454
OP 149	H2O	-513.211	Non Defined	-6.681	Non Defined
OP 150	H2O	13471.370	-11	166.427	-177.2037
OP 151	H2O	263.325	Non Defined	3.250	Non Defined
OP 152	H2O	141.698	0	1.611	-1.7248404
OP 153	H2O	-341.935	Non Defined	-4.397	Non Defined
OP 154	H2O	8975.501	-7	109.448	-116.62870
OP 155	H2O	175.444	Non Defined	2.137	Non Defined
OP 156	N2	705.203	0	0.223	-0.2227747
OP 157	N2	0.022	0	0.000	-1.667E-05
OP 158	N2	2.371	0	0.001	-0.0014773
OP 159	N2	306.857	0	0.097	-0.0969366
OP 160	N2	0.010	0	0.000	-7.257E-06
OP 161	N2	1.032	0	0.001	-0.000642
OP 162	H2	11.988	0	0.048	-0.048295
OP 163	H2	0.067	0	0.001	-0.0005528
OP 164	H2	5.216	0	0.021	-0.0210149
OP 165	H2	0.029	0	0.000	-0.000240
OP 166	O2	180.081	0	0.052	-0.0521343

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Open Path	Component	Flowrate (kg/h)	MVA (103\$/yr)	EWC (103\$/yr)	TVA(103\$/yr)
OP 167	O2	0.199	0	0.000	-0.0001361
OP 168	O2	2.380	0	0.001	-0.0013422
OP 169	O2	0.056	0	0.000	-3.184E-05
OP 170	O2	78.359	0	0.023	-0.0226853
OP 171	O2	0.087	0	0.000	-5.922E-05
OP 172	O2	1.036	0	0.001	-0.0005840
OP 173	O2	0.025	0	0.000	-1.385E-05
OP 174	BIURET	189.153	0	1.036	-1.0361123
OP 175	BIURET	0.013	0	0.000	-8.253E-05
OP 176	BIURET	0.163	0	0.001	-0.000961
OP 177	BIURET	0.789	0	0.005	-0.0046195
OP 178	BIURET	0.016	0	0.000	-3.211E-05
OP 179	BIURET	244.632	0	1.293	-1.2925912
OP 180	BIURET	0.017	0	0.000	-0.0001034
OP 181	BIURET	0.211	0	0.001	-0.0012027
OP 182	BIURET	1.020	0	0.006	-0.0057767
OP 183	BIURET	0.021	0	0.000	-3.753E-05
OP 184	BIURET	78.625	0	0.425	-0.4249558
OP 185	BIURET	0.006	0	0.000	-3.390E-05
OP 186	BIURET	0.068	0	0.000	-0.0003947
OP 187	BIURET	0.328	0	0.002	-0.0018963
OP 188	BIURET	0.007	0	0.000	-1.286E-05
OP 189	BIURET	68.014	0	0.359	-0.3593741
OP 190	BIURET	0.059	0	0.000	-0.0003344
OP 191	BIURET	0.284	0	0.002	-0.0016060
OP 192	BIURET	0.006	0	0.000	-1.043E-05

Cycle Path	Component	Flowrate (kg/h)	EWC (103\$/yr)	Cycle Path	Component	Flowrate (kg/h)	EWC (103\$/yr)
C1	NH3	23161.300	36.148	C249	N2	0.000	0.000
C2	CO2	2190.113	0.732	C250	H2	0.000	0.000
C3	CARB	30.350	0.013	C251	O2	0.000	0.000
C4	UREA	161.118	0.056	C252	BIURET	0.000	0.000
C5	H2O	3480.460	2.848	C253	NH3	0.001	0.000
C6	N2	0.000	0.000	C254	CO2	0.000	0.000
C7	H2	0.000	0.000	C255	CARB	0.002	0.000
C8	O2	0.000	0.000	C256	UREA	0.000	0.000
C9	BIURET	0.501	0.000	C257	H2O	0.072	0.001
C10	NH3	691.493	8.245	C258	N2	0.000	0.000
C11	CO2	1.977	0.002	C259	H2	0.000	0.000
C12	CARB	0.000	0.000	C260	O2	0.000	0.000
C13	UREA	0.000	0.000	C261	BIURET	0.000	0.000
C14	H2O	1574.541	5.735	C262	NH3	0.017	0.001
C15	N2	0.000	0.000	C263	CO2	0.000	0.000
C16	H2	0.000	0.000	C264	CARB	0.002	0.000
C17	O2	0.000	0.000	C265	UREA	2.112	0.016
C18	BIURET	0.000	0.000	C266	H2O	9.118	0.131
C19	NH3	20.022	0.042	C267	N2	0.000	0.000
C20	CO2	1.977	0.002	C268	H2	0.000	0.000

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Cycle Path	Component	Flowrate (kg/h)	EWC (103\$/yr)	Cycle Path	Component	Flowrate (kg/h)	EWC (103\$/yr)
C21	CARB	0.000	0.000	C269	O2	0.000	0.000
C22	UREA	0.000	0.000	C270	BIURET	0.000	0.000
C23	H2O	2.225	0.003	C271	NH3	2.266	0.078
C24	N2	0.000	0.000	C272	CO2	0.000	0.000
C25	H2	0.000	0.000	C273	CARB	1.687	0.014
C26	O2	0.000	0.000	C274	UREA	10.217	0.075
C27	BIURET	0.000	0.000	C275	H2O	158.502	2.287
C28	NH3	288.092	0.001	C276	N2	0.000	0.000
C29	CO2	0.113	0.000	C277	H2	0.000	0.000
C30	CARB	526.428	0.001	C278	O2	0.000	0.000
C31	UREA	2320.132	0.003	C279	BIURET	0.000	0.000
C32	H2O	41734.153	0.106	C280	NH3	26.061	0.871
C33	N2	0.000	0.000	C281	CO2	0.000	0.000
C34	H2	0.000	0.000	C282	CARB	0.000	0.000
C35	O2	0.000	0.000	C283	UREA	0.000	0.000
C36	BIURET	0.000	0.000	C284	H2O	3438.333	47.220
C37	NH3	2.266	0.002	C285	N2	0.000	0.000
C38	CO2	0.000	0.000	C286	H2	0.000	0.000
C39	CARB	0.395	0.000	C287	O2	0.000	0.000
C40	UREA	1.006	0.000	C288	BIURET	0.000	0.000
C41	H2O	50.854	0.038	C289	NH3	0.001	0.000
C42	N2	0.000	0.000	C290	CO2	0.000	0.000
C43	H2	0.000	0.000	C291	CARB	0.002	0.000
C44	O2	0.000	0.000	C292	UREA	0.000	0.000
C45	BIURET	0.000	0.000	C293	H2O	0.072	0.001
C46	NH3	2.988	0.007	C294	N2	0.000	0.000
C47	CO2	0.002	0.000	C295	H2	0.000	0.000
C48	CARB	0.000	0.000	C296	O2	0.000	0.000
C49	UREA	0.000	0.000	C297	BIURET	0.000	0.000
C50	H2O	0.202	0.000	C298	NH3	7.934	0.264
C51	N2	0.000	0.000	C299	CO2	0.000	0.000
C52	H2	0.000	0.000	C300	CARB	1.687	0.013
C53	O2	0.000	0.000	C301	UREA	57.363	0.403
C54	BIURET	0.000	0.000	C302	H2O	704.365	9.638
C55	NH3	2.266	0.002	C303	N2	0.000	0.000
C56	CO2	0.001	0.000	C304	H2	0.000	0.000
C57	CARB	2.947	0.001	C305	O2	0.000	0.000
C58	UREA	10.221	0.004	C306	BIURET	0.000	0.000
C59	H2O	158.502	0.119	C307	NH3	0.017	0.000
C60	N2	0.000	0.000	C308	CO2	0.000	0.000
C61	H2	0.000	0.000	C309	CARB	0.000	0.000
C62	O2	0.000	0.000	C310	UREA	0.026	0.000
C63	BIURET	0.000	0.000	C311	H2O	9.118	0.082
C64	NH3	688.525	0.392	C312	N2	0.000	0.000
C65	CO2	4.475	0.000	C313	H2	0.000	0.000
C66	CARB	0.000	0.000	C314	O2	0.000	0.000
C67	UREA	0.001	0.000	C315	BIURET	0.000	0.000
C68	H2O	1755.540	0.011	C316	NH3	0.017	0.000
C69	N2	0.000	0.000	C317	CO2	0.000	0.000

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Cycle Path	Component	Flowrate (kg/h)	EWC (103\$/yr)	Cycle Path	Component	Flowrate (kg/h)	EWC (103\$/yr)
C70	H2	0.000	0.000	C318	CARB	0.000	0.000
C71	O2	0.000	0.000	C319	UREA	0.000	0.000
C72	BIURET	0.000	0.000	C320	H2O	9.118	0.075
C73	NH3	771.116	0.439	C321	N2	0.000	0.000
C74	CO2	0.000	0.000	C322	H2	0.000	0.000
C75	CARB	0.000	0.000	C323	O2	0.000	0.000
C76	UREA	0.000	0.000	C324	BIURET	0.000	0.000
C77	H2O	8255.726	0.052	C325	NH3	0.001	0.000
C78	N2	0.000	0.000	C326	CO2	0.000	0.000
C79	H2	0.000	0.000	C327	CARB	0.000	0.000
C80	O2	0.000	0.000	C328	UREA	0.000	0.000
C81	BIURET	0.000	0.000	C329	H2O	0.072	0.001
C82	NH3	87.488	0.079	C330	N2	0.000	0.000
C83	CO2	0.064	0.000	C331	H2	0.000	0.000
C84	CARB	0.000	0.000	C332	O2	0.000	0.000
C85	UREA	0.000	0.000	C333	BIURET	0.000	0.000
C86	H2O	16.487	0.011	C334	NH3	0.017	0.000
C87	N2	0.000	0.000	C335	CO2	0.000	0.000
C88	H2	0.000	0.000	C336	CARB	0.000	0.000
C89	O2	0.000	0.000	C337	UREA	0.026	0.000
C90	BIURET	0.000	0.000	C338	H2O	9.118	0.075
C91	NH3	2.988	0.005	C339	N2	0.000	0.000
C92	CO2	0.064	0.000	C340	H2	0.000	0.000
C93	CARB	0.000	0.000	C341	O2	0.000	0.000
C94	UREA	0.000	0.000	C342	BIURET	0.000	0.000
C95	H2O	0.202	0.000	C343	NH3	1.064	0.018
C96	N2	0.000	0.000	C344	CO2	0.000	0.000
C97	H2	0.000	0.000	C345	CARB	0.000	0.000
C98	O2	0.000	0.000	C346	UREA	0.026	0.000
C99	BIURET	0.000	0.000	C347	H2O	9.518	0.078
C100	NH3	0.001	0.000	C348	N2	0.000	0.000
C101	CO2	0.000	0.000	C349	H2	0.000	0.000
C102	CARB	0.000	0.000	C350	O2	0.000	0.000
C103	UREA	0.000	0.000	C351	BIURET	0.000	0.000
C104	H2O	0.072	0.000	C352	NH3	1.064	0.017
C105	N2	0.000	0.000	C353	CO2	0.000	0.000
C106	H2	0.000	0.000	C354	CARB	0.000	0.000
C107	O2	0.000	0.000	C355	UREA	0.000	0.000
C108	BIURET	0.000	0.000	C356	H2O	9.518	0.071
C109	NH3	0.001	0.000	C357	N2	0.000	0.000
C110	CO2	0.000	0.000	C358	H2	0.000	0.000
C111	CARB	0.000	0.000	C359	O2	0.000	0.000
C112	UREA	0.000	0.000	C360	BIURET	0.000	0.000
C113	H2O	0.202	0.000	C361	NH3	0.001	0.000
C114	N2	0.000	0.000	C362	CO2	0.000	0.000
C115	H2	0.000	0.000	C363	CARB	0.000	0.000
C116	O2	0.000	0.000	C364	UREA	0.000	0.000
C117	BIURET	0.000	0.000	C365	H2O	0.072	0.001
C118	NH3	2.988	0.005	C366	N2	0.000	0.000

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Cycle Path	Component	Flowrate (kg/h)	EWC (103\$/yr)	Cycle Path	Component	Flowrate (kg/h)	EWC (103\$/yr)
C119	CO2	0.007	0.000	C367	H2	0.000	0.000
C120	CARB	0.000	0.000	C368	O2	0.000	0.000
C121	UREA	0.000	0.000	C369	BIURET	0.000	0.000
C122	H2O	0.202	0.000	C370	NH3	1.064	0.017
C123	N2	0.000	0.000	C371	CO2	0.000	0.000
C124	H2	0.000	0.000	C372	CARB	0.000	0.000
C125	O2	0.000	0.000	C373	UREA	0.026	0.000
C126	BIURET	0.000	0.000	C374	H2O	9.518	0.071
C127	NH3	0.000	0.000	C375	N2	0.000	0.000
C128	CO2	0.000	0.000	C376	H2	0.000	0.000
C129	CARB	0.000	0.000	C377	O2	0.000	0.000
C130	UREA	0.201	0.002	C378	BIURET	0.000	0.000
C131	H2O	18.904	0.302	C379	NH3	2.266	0.036
C132	N2	0.000	0.000	C380	CO2	0.000	0.000
C133	H2	0.000	0.000	C381	CARB	0.001	0.000
C134	O2	0.000	0.000	C382	UREA	6.897	0.023
C135	BIURET	0.000	0.000	C383	H2O	158.502	1.167
C136	NH3	0.000	0.000	C384	N2	0.000	0.000
C137	CO2	0.000	0.000	C385	H2	0.000	0.000
C138	CARB	0.000	0.000	C386	O2	0.000	0.000
C139	UREA	0.000	0.000	C387	BIURET	0.000	0.000
C140	H2O	18.904	0.289	C388	NH3	387.769	5.854
C141	N2	0.000	0.000	C389	CO2	0.000	0.000
C142	H2	0.000	0.000	C390	CARB	0.000	0.000
C143	O2	0.000	0.000	C391	UREA	0.000	0.000
C144	BIURET	0.000	0.000	C392	H2O	5020.386	33.460
C145	NH3	0.000	0.000	C393	N2	0.000	0.000
C146	CO2	0.000	0.000	C394	H2	0.000	0.000
C147	CARB	0.000	0.000	C395	O2	0.000	0.000
C148	UREA	0.000	0.000	C396	BIURET	0.000	0.000
C149	H2O	0.072	0.001	C397	NH3	0.001	0.000
C150	N2	0.000	0.000	C398	CO2	0.000	0.000
C151	H2	0.000	0.000	C399	CARB	0.001	0.000
C152	O2	0.000	0.000	C400	UREA	0.000	0.000
C153	BIURET	0.000	0.000	C401	H2O	0.072	0.000
C154	NH3	0.000	0.000	C402	N2	0.000	0.000
C155	CO2	0.000	0.000	C403	H2	0.000	0.000
C156	CARB	0.000	0.000	C404	O2	0.000	0.000
C157	UREA	0.201	0.002	C405	BIURET	0.000	0.000
C158	H2O	18.904	0.288	C406	NH3	7.934	0.119
C159	N2	0.000	0.000	C407	CO2	0.000	0.000
C160	H2	0.000	0.000	C408	CARB	0.001	0.000
C161	O2	0.000	0.000	C409	UREA	6.897	0.020
C162	BIURET	0.000	0.000	C410	H2O	704.365	4.659
C163	NH3	0.003	0.000	C411	N2	0.000	0.000
C164	CO2	0.000	0.000	C412	H2	0.000	0.000
C165	CARB	0.023	0.000	C413	O2	0.000	0.000
C166	UREA	10.217	0.080	C414	BIURET	0.000	0.000
C167	H2O	264.572	4.030	C415	NH3	22.013	0.304

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Cycle Path	Component	Flowrate (kg/h)	EWC (103\$/yr)	Cycle Path	Component	Flowrate (kg/h)	EWC (103\$/yr)
C168	N2	0.000	0.000	C416	CO2	0.000	0.000
C169	H2	0.000	0.000	C417	CARB	0.000	0.000
C170	O2	0.000	0.000	C418	UREA	0.000	0.000
C171	BIURET	0.000	0.000	C419	H2O	50.854	0.258
C172	NH3	0.003	0.000	C420	N2	0.000	0.000
C173	CO2	0.000	0.000	C421	H2	0.000	0.000
C174	CARB	0.000	0.000	C422	O2	0.000	0.000
C175	UREA	0.000	0.000	C423	BIURET	0.000	0.000
C176	H2O	264.572	3.846	C424	NH3	0.001	0.000
C177	N2	0.000	0.000	C425	CO2	0.000	0.000
C178	H2	0.000	0.000	C426	CARB	0.001	0.000
C179	O2	0.000	0.000	C427	UREA	0.000	0.000
C180	BIURET	0.000	0.000	C428	H2O	0.072	0.000
C181	NH3	0.001	0.000	C429	N2	0.000	0.000
C182	CO2	0.000	0.000	C430	H2	0.000	0.000
C183	CARB	0.002	0.000	C431	O2	0.000	0.000
C184	UREA	0.000	0.000	C432	BIURET	0.000	0.000
C185	H2O	0.072	0.001	C433	NH3	7.934	0.109
C186	N2	0.000	0.000	C434	CO2	0.000	0.000
C187	H2	0.000	0.000	C435	CARB	0.001	0.000
C188	O2	0.000	0.000	C436	UREA	1.006	0.002
C189	BIURET	0.000	0.000	C437	H2O	50.854	0.256
C190	NH3	0.003	0.000	C438	N2	0.000	0.000
C191	CO2	0.000	0.000	C439	H2	0.000	0.000
C192	CARB	0.023	0.000	C440	O2	0.000	0.000
C193	UREA	23.609	0.175	C441	BIURET	0.000	0.000
C194	H2O	264.572	3.833	C442	NH3	668.207	9.166
C195	N2	0.000	0.000	C443	CO2	0.000	0.000
C196	H2	0.000	0.000	C444	CARB	0.001	0.000
C197	O2	0.000	0.000	C445	UREA	2.909	0.006
C198	BIURET	0.000	0.000	C446	H2O	1256.654	6.313
C199	NH3	0.048	0.002	C447	N2	0.000	0.000
C200	CO2	0.000	0.000	C448	H2	0.000	0.000
C201	CARB	0.310	0.003	C449	O2	0.000	0.000
C202	UREA	10.217	0.076	C450	BIURET	0.020	0.000
C203	H2O	158.502	2.297	C451	NH3	289.356	3.999
C204	N2	0.000	0.000	C452	CO2	0.000	0.000
C205	H2	0.000	0.000	C453	CARB	0.000	0.000
C206	O2	0.000	0.000	C454	UREA	0.000	0.000
C207	BIURET	0.000	0.000	C455	H2O	407.790	2.071
C208	NH3	0.048	0.002	C456	N2	0.000	0.000
C209	CO2	0.000	0.000	C457	H2	0.000	0.000
C210	CARB	0.000	0.000	C458	O2	0.000	0.000
C211	UREA	0.000	0.000	C459	BIURET	0.000	0.000
C212	H2O	502.771	6.937	C460	NH3	0.001	0.000
C213	N2	0.000	0.000	C461	CO2	0.000	0.000
C214	H2	0.000	0.000	C462	CARB	0.001	0.000
C215	O2	0.000	0.000	C463	UREA	0.000	0.000
C216	BIURET	0.000	0.000	C464	H2O	0.072	0.000

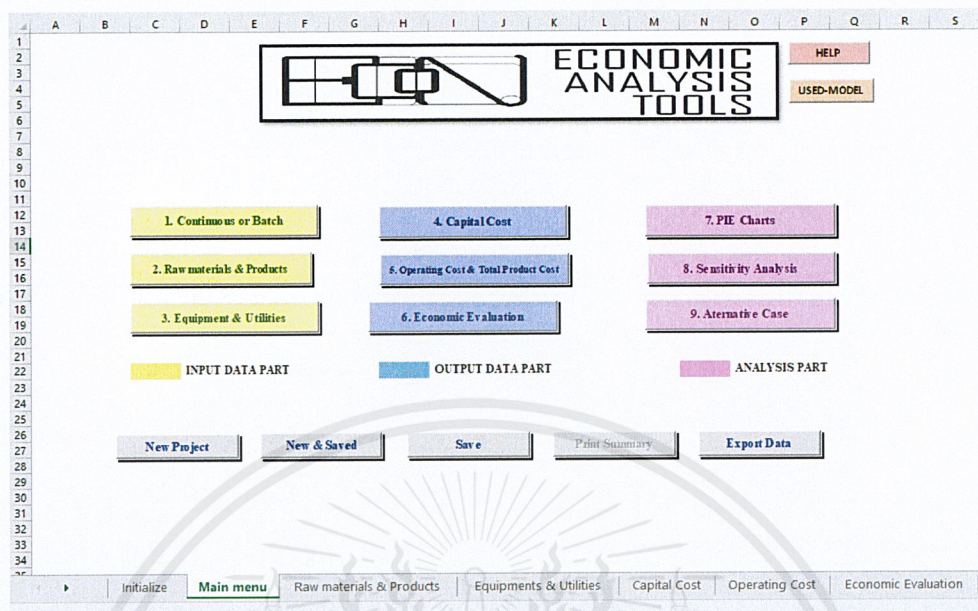
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Cycle Path	Component	Flowrate (kg/h)	EWC (103\$/yr)	Cycle Path	Component	Flowrate (kg/h)	EWC (103\$/yr)
C217	NH3	0.001	0.000	C465	N2	0.000	0.000
C218	CO2	0.000	0.000	C466	H2	0.000	0.000
C219	CARB	0.002	0.000	C467	O2	0.000	0.000
C220	UREA	0.000	0.000	C468	BIURET	0.000	0.000
C221	H2O	0.072	0.001	C469	NH3	7.934	0.109
C222	N2	0.000	0.000	C470	CO2	0.000	0.000
C223	H2	0.000	0.000	C471	CARB	0.001	0.000
C224	O2	0.000	0.000	C472	UREA	2.909	0.006
C225	BIURET	0.000	0.000	C473	H2O	407.790	2.050
C226	NH3	0.048	0.002	C474	N2	0.000	0.000
C227	CO2	0.000	0.000	C475	H2	0.000	0.000
C228	CARB	0.310	0.002	C476	O2	0.000	0.000
C229	UREA	57.363	0.404	C477	BIURET	0.000	0.000
C230	H2O	502.771	6.912	C478	NH3	5097.638	8.864
C231	N2	0.000	0.000	C479	CO2	1125.135	0.452
C232	H2	0.000	0.000	C480	CARB	0.000	0.000
C233	O2	0.000	0.000	C481	UREA	0.000	0.000
C234	BIURET	0.000	0.000	C482	H2O	775.832	0.708
C235	NH3	0.017	0.001	C483	N2	28.968	0.004
C236	CO2	0.000	0.000	C484	H2	0.716	0.001
C237	CARB	0.002	0.000	C485	O2	27.737	0.004
C238	UREA	2.112	0.016	C486	BIURET	0.000	0.000
C239	H2O	9.118	0.138	C487	NH3	692.122	1.080
C240	N2	0.000	0.000	C488	CO2	24.645	0.008
C241	H2	0.000	0.000	C489	CARB	4382.125	1.863
C242	O2	0.000	0.000	C490	UREA	542.297	0.189
C243	BIURET	0.000	0.000	C491	H2O	523.884	0.429
C244	NH3	0.017	0.001	C492	N2	0.000	0.000
C245	CO2	0.000	0.000	C493	H2	0.000	0.000
C246	CARB	0.000	0.000	C494	O2	0.000	0.000
C247	UREA	0.000	0.000	C495	BIURET	0.000	0.000
C248	H2O	9.118	0.132				

B. Economic analysis

ECON software



Utility cost evaluation

No.	EQUIPMENT	Utility	UTILITY COST (\$/hr)		
			Base case design	Alternative 1	Alternative 2
E-1	Heat Exchanger	Cooling water	5.03699311	22.02725292	19.34670304
E-2	Heat Exchanger	Cooling water	3.75877558	3.758775577	3.758775577
E-3	Heat Exchanger	Cooling water	13.7504012	-	-
E-4	Heat Exchanger	Cooling water	6.8145916		
E-5	Heat Exchanger	Cooling water	3.58102813		
E-6	Heat Exchanger	Cooling water	23.4347164		
E-7	Heat Exchanger	Cooling water	10.3720407	3.31478417	16.07585
E-8	Heat Exchanger	Cooling water	4.84937613		
E-9	Heat Exchanger	Cooling water	0.52744126		
E-10	Heat Exchanger	Cooling water	0.59748886	0.260484362	0.285896633
E-11	Heat Exchanger	Cooling water	0.01959436	0.020723601	0.020487716
E-12	Heat Exchanger	Cooling water	10.2016378	10.3747135	10.57982517
T-1	Tower Unit	Cooling water	7.0527366	7.052736605	7.052736605
T-3	Tower Unit	MP utility	283.230022	287.3331555	593.4909851
T-5	Tower Unit	MP utility	102.919042	-	-
T-6	Tower Unit	MP utility	553.283929	-	-
T-7	Tower Unit	MP utility	2.3059997	8.104541702	199.1218947
R-1	Reactor	Cooling water	56.0636002	53.10028223	53.54946106
C-1	Compressor	Electricity	393.212694	393.2126944	393.2126944
C-2	Compressor	Electricity	171.09989	171.0998897	171.0998897
P-1	Pump	Electricity	15.8464205	15.84642048	15.84642048
P-2	Pump	Electricity	9.7096227	9.9732945	9.21977472

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No.	EQUIPMENT	Utility	UTILITY COST (\$/hr)		
			Base case design	Alternative 1	Alternative 2
P-3	Pump	Electricity	0.04446412	0.007932033	0.007815477
P-4	Pump	Electricity	0.06180775	0.061807747	0.061807747
P-5	Pump	Electricity	0.02946804	0.030785485	0.030331807
P-6	Pump	Electricity	0.11003031	0.114949492	0.11325551
P-7	Pump	Electricity	0.45691886	-	-
P-8	Pump	Electricity	0.26316883	0.188620183	0.183241531
P-9	Pump	Electricity	1.14885702	0.790130676	0.782511312
P-10	Pump	Electricity	0.03943721	0.045072049	0.043601898

C. LCA analysis

Emission factor

CO2eq Emissions	kg/GJ	kg/kWh
District Steam and Hot water	56.753	
District Chilled Water - Engine-Driven Chiller Natural Gas	13.760	
Electricity		0.283

Carbon footprint results

Unit	Type of unit	Activity	Carbon Footprint (CO2 eq.)		
			Base Case design	Alternative 1	Alternative 2
E-1	Heat Exchanger	Cooling	0.002579	0.011085	0.009718
E-2	Heat Exchanger	Cooling	0.001925	0.001892	0.001888
E-3	Heat Exchanger	Cooling	0.007041	-	-
E-4 - E-9	Heat Exchanger	Cooling	0.025386	0.001668	0.008075
E-10	Heat Exchanger	Cooling	0.000306	0.000131	0.000144
E-11	Heat Exchanger	Cooling	0.000010	0.000010	0.000010
E-12	Heat Exchanger	Cooling	0.005223	0.005221	0.005314
T-1	Tower Unit	Cooling	0.003611	0.003549	0.003543
T-3	Tower Unit	Heating	0.025468	0.025394	0.025355
T-5	Tower Unit	Heating	0.009255	-	-
T-6	Tower Unit	Heating	0.049751	-	-
T-7	Tower Unit	Heating	0.000207	0.000716	0.017566
R-1	Reactor	Cooling	0.028706	0.026723	0.026899
C-1	Compressor	Electric usage	0.028015	0.027535	0.027484
C-2	Compressor	Electric usage	0.012190	0.011981	0.011959
P-1	Pump	Electric usage	0.000974	0.000957	0.000955
P-2	Pump	Electric usage	0.000597	0.000602	0.000556
P-3	Pump	Electric usage	2.73207E-06	4.79025E-07	4.71115E-07

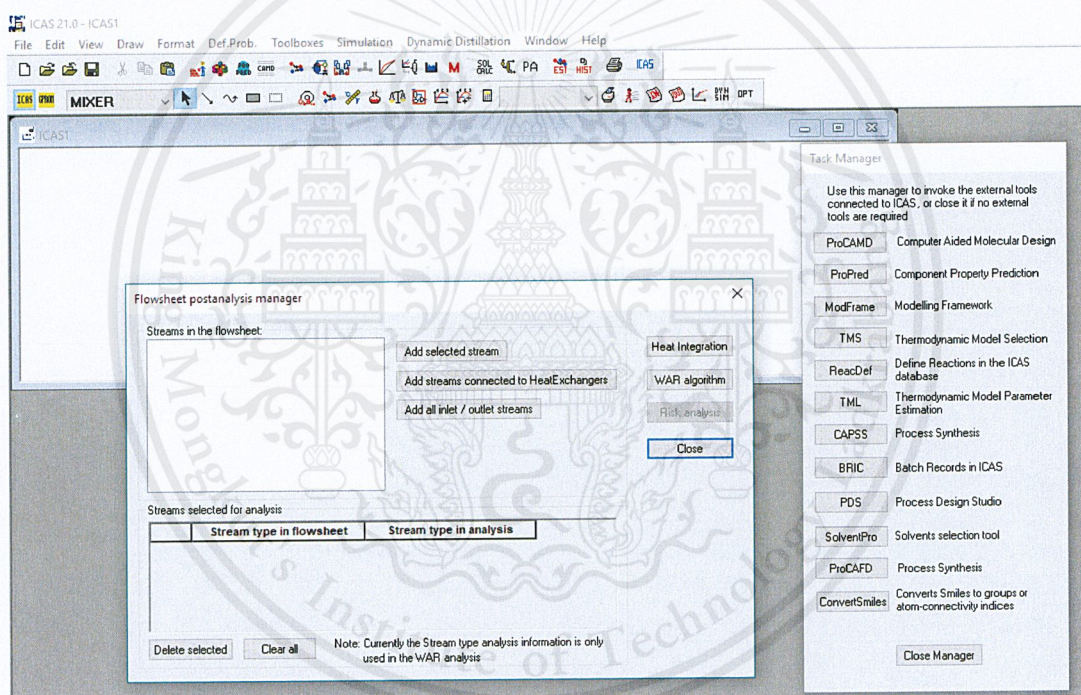
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Unit	Type of unit	Activity	Carbon Footprint (CO ₂ eq.)		
			Base Case design	Alternative 1	Alternative 2
P-4	Pump	Electric usage	3.79774E-06	3.73265E-06	3.72576E-06
P-5	Pump	Electric usage	1.81064E-06	1.85917E-06	1.82839E-06
P-6	Pump	Electric usage	6.76074E-06	6.94194E-06	6.82702E-06
P-7	Pump	Electric usage	2.80751E-05	-	-
P-8	Pump	Electric usage	1.61702E-05	1.1391E-05	1.10458E-05
P-9	Pump	Electric usage	7.05908E-05	4.7717E-05	4.71696E-05
P-10	Pump	Electric usage	2.42319E-06	2.72196E-06	2.62831E-06

D. Waste reduction (WAR) algorithm analysis

ICAS software



WAR algorithm results

- ATP - Aquatic Toxicity Potential (1/L50)
- HTPI - Human Toxicity Potential by Ingestion (1/L50)
- TTP - Terrestrial Toxicity Potential (1/L50)
- HTPE - Human Toxicity Potential by Exposure (mg emission/m³)
- GWP - Global Warming Potential (CO₂ eq.)
- AP - Acidification Potential (H⁺ eq.)

	Base case design		
	Input sum	Output sum	Impact generated
HTPI	44886.38	4004.7	-40881.68
HTPE	380.07	23.45	-356.62
ATP	7929.03	141.2	-7787.83
TTP	44886.38	4004.7	-40881.68
GWP	18.33	0.3	-18.03
AP	81857.77	1484.47	-80373.3

	Alternative 1		
	Input sum	Output sum	Impact generated
HTPI	44886.38	3389.39	-41497
HTPE	380.07	18.05	-362.02
ATP	7929.03	24.09	-7904.94
TTP	44886.38	3389.39	-41497
GWP	18.33	0.04	-18.29
AP	81857.77	261.1	-81596.7

	Alternative 2		
	Input sum	Output sum	Impact generated
HTPI	44886.38	3297.41	-41589
HTPE	380.07	17.25	-362.82
ATP	7929.03	6.53	-7922.5
TTP	44886.38	3297.41	-41589
GWP	18.33	0	-18.33
AP	81857.77	82.44	-81775.3

E. Properties of pure compounds

Com- pound	MW (g/mol)	Tm (K)	Tb (K)	Solubility parameter (MPa ^{0.5})	Radius of gyra- tion (A)	VdW m ³ /kmol	VM m ³ /kmol	VP atm (@298K)
NH3	17.03	195.41	239.72	29.23	0.85	0.0138	0.0250	NA
CO2	44.01	216.58	185.16	14.56	1.04	0.0197	0.0373	NA
CARB	78.07	333	636.84	NA	NA	0.0319	0.0587	1.6E-08
UREA	60.06	405.85	465	36.24	2.6	0.0323	0.0488	2.69E-06
H2O	18.01	273.15	373.15	47.81	0.62	0.0124	0.0181	0.0309
N2	28.01	63.15	77.34	9.08	0.55	0.0158	0.0347	NA
H2	2.02	13.95	20.39	6.65	0.37	0.0063	0.0286	NA
O2	32.00	54.36	90.19	8.18	0.68	0.013	0.0280	NA
BIURET	103.08	470.72	725.47	38.42	NA	0.0456	0.1566	3.27E-09

Biography

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